

3.0 WASTE AND CONSTITUENT PARAMETERS

This section discusses the individual waste and constituent parameters required to perform a modeling analysis using EPACMTP. Each of the input parameters describing the waste and constituent can be specified as a constant value or as a statistical or empirical distribution of values. As a practical matter, however, many of these inputs are commonly set to constant values.

When modeling a WMU using a pulse source term (typically done for the SI, WP, and LAU scenario), the only waste-specific input parameter required by the model is the leachate concentration. When modeling a LF, the waste volume, waste density and the waste concentration are also needed by the model (For a complete listing of the LF source term variables, see Section 2.2.1 of the *EPACMTP Technical Background Document*). These additional waste parameters are used to determine the amount of constituent in the landfill that is available for leaching. The waste volume is entered in EPACMTP in terms of a fraction of the entire LF volume, and is discussed in Section 2 of this document, under the source parameters.

The constituent-specific parameters are used to simulate the chemical fate of constituents as they are transported through the subsurface; these inputs can be divided into three categories:

- 1) General and Constitutive Input Parameters
 - e.g., molecular weight, molecular diffusion, and regulatory standard in drinking water.
- 2) Organic Constituent Specific Input Parameters
 - to describe the tendency of the constituent to degrade to form harmless and/or toxic degradation products; and
 - to quantify the capacity of the constituent to adsorb to the organic components of the soil matrix.
- 3) Non-Linear Metal Constituent Geochemical Input Parameters
 - to determine the mobility of a metal constituent in the subsurface.

The EPACMTP model simulates the ground-water fate and transport of waste constituents by using these constituent-specific parameters in conjunction with the properties of the subsurface.

The waste and constituent parameters are individually described in the following sections.

3.1 WASTE AND CONSTITUENT PARAMETERS

The input parameters used in EPACMTP to describe the modeled waste and constituent are listed in Table 3.1.

Table 3.1 Waste and Constituent Parameters

Parameter Type	Parameter	Symbol	Units	Section	Equation in EPACMTP TBD
Waste	Waste Density	ρ_{hw}	g/cm ³	3.2.1	2.3
	Waste Concentration (conc. of constituent in Waste)	C_w	mg/kg	3.2.2	2.3
	Leachate Concentration (conc. of constituent in leachate)	C_L	mg/L	3.2.3	2.1
All Constituents	Molecular Diffusion Coefficient	D_i	m ² /yr	3.3.1.1	3.15
	Drinking Water Standard	DWS	mg/L	3.3.1.2	
	Molecular Weight	MW	g/mol	3.3.1.3	4.37
Organic Constituents	Organic Carbon Partition Coefficient	k_{oc}	cm ³ /g	3.3.2.1	2.29
	Dissolved Phase Hydrolysis Decay Rate	λ_1	1/yr	3.3.2.2.1	3.13
	Sorbed Phase Hydrolysis Decay Rate	λ_2	1/yr	3.3.2.2.2	3.13
	Acid-Catalyzed Hydrolysis Rate Constant	K_a^{Tr}	1/(mol.yr)	3.3.2.2.3	
	Neutral Hydrolysis Rate Constant	K_n^{Tr}	1/yr	3.3.2.2.4	
	Base-Catalyzed Hydrolysis Rate Constant	K_b^{Tr}	1/(mol.yr)	3.3.2.2.5	
	Hydrolysis Reference Temperature	T_r	°C	3.3.2.2.6	
Transformation Products	Degradation Species Number	ℓ	unitless	3.3.2.3.1	4.31
	Number of Immediate Parents	M_i	unitless	3.3.2.3.2	4.31
	Species Number of Immediate Parent	m_i	unitless	3.3.2.3.3	4.31
	Speciation Factor	ξ_{im}	unitless	3.3.2.3.4	4.31

Table 3.1 Waste and Constituent Parameters (continued)

Parameter Type	Parameter	Symbol	Units	Section	Equation in EPACMTP TBD
Metal Constituents	Metal Identification Number	ID	unitless	3.3.3.2.1	Section G.4.1.2 (Appendix G)
	Soil and Aquifer pH	pH	standard units	3.3.3.2.2	Section G.4.1.2 (Appendix G)
	Iron Hydroxide Content	FeOx	wt % Fe	3.3.3.2.3	Section G.4.1.2 (Appendix G)
	Leachate Organic Acid Concentration	LOM	mol/L	3.3.3.2.4	Section G.4.1.2 (Appendix G)
	Percent Organic Matter	%OM	unitless	3.3.3.2.5	Section G.4.1.2 (Appendix G)
	Fraction Organic Carbon	f_{oc}	unitless	3.3.3.2.6	Section G.4.1.2 (Appendix G)
	Ground-water Type (carbonate/non-carbonate)	IGWT	unitless	3.3.3.2.7	Section G.4.1.2 (Appendix G)

3.2 WASTE CHARACTERISTICS

3.2.1 Waste Density (ρ_{hw})

Definition

The waste density is defined as the average wet bulk density of the waste, i.e., mass of waste per unit volume (kg/L or g/cm³) containing the constituent(s) of concern and should be measured on the waste as disposed, as opposed to a dry bulk density. This parameter is only used when modeling landfills.

Parameter Value or Distribution of Values

Information on the density of hazardous waste was developed using the densities of 4 major categories of waste (solvents, paints, petroleum products, pesticides) and their contributions to the composition of hazardous wastes in Subtitle D landfills (Schanz and Salhotra, 1992). The results are expressed as an empirical distribution of waste densities, given in Table 3.2. The default distribution shows a relatively narrow range of variation, from 0.7 to 2.1 g/cm³.

For waste-specific applications of EPACMTP, it is recommended to use appropriate waste-specific data, rather than the default distribution.

Table 3.2 Default Cumulative probability distribution of waste density

Waste Density (g/cm ³)	Cumulative Probability
0.7	0
0.9	0.530
1.12	0.550
1.13	0.551
1.28	0.553
1.30	0.640
1.33	0.728
1.34	0.815
1.36	0.826
1.46	0.904
1.50	0.905
1.62	0.906
1.63	0.994
1.64	0.995
1.65	0.996
2.10	0.998

Data Sources

The default data presented in Table 3.2 were developed by Schanz and Salhotra (1992).

Use In EPACMTP

When modeling a landfill, the EPACMTP model uses the waste density to convert between waste volume and mass; the total mass of the waste in the landfill is then used in conjunction with the waste concentration to derive the contaminant mass available to be leached to the subsurface.

3.2.2 Concentration of Constituent in the Waste (C_w)

Definition

The waste concentration (mg/kg) represents the total fraction of constituent in the waste which may eventually leach out. Strictly speaking, C_w is the total leachable waste concentration. However, from a practical perspective, C_w may be interpreted to represent the total waste concentration and measured accordingly. This approach will be protective because the measured total waste concentration should always be at least as high as the more difficult to quantify "leachable" waste concentration.

The waste concentration used by EPACMTP reflects the average concentration of the constituent(s) of concern in the waste in the WMU at the time of closure. Contaminant losses that may occur during the WMU's active life are not explicitly modeled in EPACMTP. If such losses are significant, it may be appropriate to adjust the waste concentration accordingly (see Section 3.2.4) to represent the remaining constituent concentration available for leaching. However, ignoring these other loss pathways will be protective for the ground-water pathway analysis.

Parameter Value or Distribution of Values

The waste concentration is waste- and constituent-specific. There is no default value or distribution for this parameter.

Data Sources

There is no default value or distribution for this parameter. Waste-specific data should be obtained from appropriate chemical analytical tests on the waste of interest.

Use In EPACMTP

EPACMTP uses the waste concentration to calculate the contaminant mass within the landfill; the contaminant mass is an important input for determining the landfill leaching duration (see Section 2.2.1.3.3 of the *EPACMTP Technical Background Document*; U.S. EPA, 2003a).

3.2.3 Concentration of Constituent in the Leachate (C_L)

Definition

The leachate concentration (mg/L) is the mass of the dissolved constituent per unit volume of water emanating from the base of the WMU. This parameter provides the boundary condition for the EPACMTP simulation of constituent fate and transport through the unsaturated and saturated zone. For a continuous or pulse source, this concentration is constant until leaching stops. For the landfill depleting source option, the initial leaching concentration value must be provided by the user as an EPACMTP input parameter; the model then automatically adjusts the value as the waste is depleted during the simulation.

Parameter Value or Distribution of Values

The leachate concentration is waste- and constituent-specific. There is no default value or distribution for this parameter.

EPACMTP can accommodate a measured value or distribution of values, as determined from an appropriate leaching test procedure such as the Toxicity

Characteristic Leaching Procedure (TCLP) or the Synthetic Precipitation Leaching Procedure.¹

If EPACMTP is used to back-calculate a loading or leaching risk-based or regulatory limit for organic constituents (that is, the DAF is the only required model output), then the leachate concentration value that is used as an EPACMTP input is not material and an arbitrary value, such as 1×10^6 mg/L, can be used. However, if a forward risk analysis is being performed for an organic constituent (when the magnitude of the receptor well concentration is being determined to calculate risk), then actual analytical concentration(s) is/are used as input to the EPACMTP model.

On the other hand, if the constituent of interest is a metal or inorganic with a nonlinear sorption isotherm, then the actual value of the leachate concentration is material to the analysis, no matter if the goal is to calculate risk based on the resulting receptor well concentration (a forward risk calculation) or to determine a threshold waste or leachate concentration based on a defined risk level (a backward risk calculation). The reason for this is that the nonlinear isotherms which can be used to model the adsorption of metals mean that there is a nonlinear relationship between the input leachate concentration and the resulting receptor well concentration. That is, for metals, we can't calculate a DAF that is constant across all leachate concentrations. So, even when the goal of the analysis is to determine an allowable threshold concentration for a metal constituent (a backward risk calculation), the leachate concentration is an important model input. Such an analysis will typically require repeated simulations, each with a different leachate concentration, until the leachate concentration is identified that results in the receptor well concentration being equal to a given regulatory or risk-based benchmark concentration. Additionally, when we perform an EPACMTP analysis for use in a forward risk calculation for metal constituents, actual analytical concentrations are typically used as input to the EPACMTP model to determine the resulting risk.

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Remember that the DAF is calculated by dividing the input leachate concentration by the resulting receptor well concentration. Since the ground-water transport for organic constituents is linear, if all other model inputs are held constant and the input leachate concentration is doubled, the receptor well concentration will be doubled – but the DAF will remain the same. For this reason, if EPACMTP is being used to back-calculate a threshold waste or leachate concentration, the input leachate concentration for an organic constituent is arbitrary. The value of 1×10^6 mg/L is commonly used for this arbitrary concentration simply because its large value makes insignificant any errors due to numerical oscillations in the transport solution.

Data Sources

The waste concentration is waste- and constituent-specific. There is no default value or distribution for this parameter.

Use In EPACMTP

The EPACMTP fate and transport model requires stipulation of the leachate concentration as a function of time, $C_L(t)$. The leachate concentration $C_L(t)$ used in the model directly represents the concentration of the leachate emanating from the base of the waste management unit, as a boundary condition for the numerical fate and transport model. EPACMTP accounts for time variation as either a constant concentration pulse condition, or as an exponentially decreasing leachate concentration (depleting source).

In the finite source option, the simplest and generally most conservative case is to assume that the leachate concentration remains constant until all of the initially present contaminant mass has leached out of the disposal unit. This case is referred to as the pulse (or non-depleting) source scenario. The boundary condition for the fate and transport model then becomes a constant concentration pulse, with defined duration.

A more realistic modeling analysis in the case of a closed landfill with no continued waste addition to the unit, can be conducted by assuming that linear equilibrium partitioning between the solid and liquid phase of the waste leads to an exponential decrease in the leachate concentration over time as a result of depletion of the source. When using this depleting source option, the user specifies the initial leaching concentration, and the model automatically adjusts this rate over time (except for organics with nonlinear isotherms) as explained in Section 2.2.1.3.3 of the *EPACMTP Technical Background Document* (U.S. EPA, 2003a).

3.3 CONSTITUENT PHYSICAL AND CHEMICAL CHARACTERISTICS

3.3.1 All Constituents

The molecular diffusion coefficient and the molecular weight are constituent-specific inputs required by the model for all types of constituents and modeling analyses. In addition, if a finite source analysis is performed, then a value is required for the applicable drinking water standard for each constituent.

EPACMTP also accounts for constituent-specific transformation and sorption processes. These are discussed in Sections 3.3.2 and 3.3.3 for organic and metal constituents, respectively.

3.3.1.1 Molecular Diffusion Coefficient (D)

Definition

Diffusion is defined as the movement of constituent molecules in an environmental medium from areas of high constituent concentrations toward areas with lower constituent concentrations. This process occurs as a result of concentration gradients. Diffusion can occur both in the absence or presence of advective flow. In ground-water flow systems, the process of diffusion is quantified using the diffusion coefficient of the constituent and the concentration gradient of the constituent in ground water.

The coefficient of molecular diffusion is often negligible compared to the dispersivity term in the calculation of the dispersion coefficient and is commonly ignored. However, diffusion can be significant in cases where ground-water velocity is very low.

Parameter Value or Distribution of Values

The molecular diffusion coefficient is a constituent-specific input parameter and should be calculated by the user based on the molecular diffusion coefficient in free water. Molecular diffusion coefficient values for some common organic constituents are included in Appendix C. If data are not available for the modeled constituent, this parameter should be set to zero.

Data Sources

The molecular diffusion coefficient values listed in Appendix C were generated using the Water 9 model (U.S. EPA, 2001b).

Use In EPACMTP

Hydrodynamic dispersion and molecular diffusion are used to calculate the dispersion coefficient, one of the variables in the transport equation (see Section 4.4 of the *EPACMTP Technical Background Document*, U.S. EPA, 2000a).

3.3.1.2 Drinking Water Standard (DWS)

Definition

The drinking water standard (mg/L) is the level assumed to be protective. It may be a Maximum Contaminant Level (MCL) or a health-based number (HBN) (See Section 5.0 of the *IWEM Technical Background Document*, U.S. EPA, 2003c)

Parameter Value or Distribution of Values

The drinking water standard is a constituent-specific input parameter; the appropriate value must be determined by the user. The default value for this parameter is zero. The drinking water standard must be expressed in the same units used for the leachate concentration, usually mg/L. Although a distribution of values could be used for this input parameter, it is typically specified as a constant value.

Data Sources

Current values for MCLs can be obtained from the EPA's Office of Ground Water and Drinking Water (<http://www.epa.gov>). See Section 5 of the *IWEM Technical Background Document*, U.S. EPA, 2003c for a discussion of sources for HBN values.

Use In EPACMTP

The drinking water standard is used in finite source scenarios when the depleting landfill source option is invoked to determine the duration of the exponentially decaying concentration boundary condition (t_p). Leaching is assumed to continue until the constituent concentration in the leachate has dropped below the drinking water standard. The leaching duration, t_p , is determined by setting Equation 2.12 in the EPACMTP Technical Background Document (U.S. EPA, 2003a) equal to the DWS and solving for t (time).

3.3.1.3 Molecular Weight (MW)***Definition***

The molecular weight (g/mol) is defined as the amount of mass in one mole of molecules of a constituent as determined by summing the atomic weights of the elements in that constituent, multiplied by their stoichiometric factors.

Parameter Value or Distribution of Values

The molecular weight is a constituent-specific input parameter; the appropriate value must be provided by the user. There is no default value.

Data Sources

Compilations of chemical data such as molecular weight are available on many web sites and in most chemistry reference books.

Use In EPACMTP

The use of this parameter is reserved for future versions of EPACMTP to automatically calculate the parent to degradation product yield or decay coefficients for chain decay simulations.

3.3.2 Organic Constituents

This section describes the parameters used in EPACMTP for organic constituents. The parameters to be discussed are the organic carbon partition coefficient, sorbed and dissolved phase hydrolysis decay rate, acid, neutral, and base-catalyzed hydrolysis rate constants, and the reference temperature.

For organic constituents, EPACMTP takes into account adsorption behavior of organic constituents by calculating a retardation factor based on the organic carbon distribution coefficient (k_{oc}) of each constituent and fractional organic carbon in the soil (f_{oc}) (See Section 3.2.1).

In order to model the subsurface fate and transport of organic constituents, EPACMTP generates a single first-order degradation rate, which includes both biodegradation and chemical hydrolysis (in both sorbed and dissolved phases). The biodegradation rate is typically set to zero (due to the difficulty in accurately estimating it), but a non-zero value can be specified by the user. The user can directly specify the hydrolysis rates, or they can be internally calculated by the model (see Section 3.3.2.2). If calculated, EPACMTP requires that the hydrolysis rate constants and the reference temperature at which they were measured be specified. EPACMTP then uses these rate constants along with the ground-water temperature and pH to derive the sorbed-phase and dissolved-phase hydrolysis rates. These two hydrolysis rates and the biodegradation rate (if non-zero) are then combined into the overall first-order degradation rate. If the products of this degradation are themselves toxic, they can be included in the modeling analysis by specifying them to be part of a decay chain, with the current organic constituent as the parent chemical.

If desired, the user can override the default of no biodegradation, by providing appropriate values of the biodegradation rate coefficient for the unsaturated and saturated zone (see Section 5 of this document).

3.3.2.1 Organic Carbon Partition Coefficient (k_{oc})

Definition

The organic carbon partition coefficient (cm^3/g) is the ratio of a constituent's concentration in a theoretical soil containing only organic carbon to its concentration in the ground water. Thus, k_{oc} describes the affinity of a constituent to attach itself to organic carbon. This parameter is applicable to organic constituents which tend to sorb onto the organic matter in soil or in an aquifer. Constituents with high k_{oc} values tend to move more slowly through the soil and ground water. Volatile organics tend to have low k_{oc} values, whereas semi-volatile organics often have high k_{oc} values.

Parameter Value or Distribution of Values

The organic carbon partition coefficient is a constituent-specific input parameter; values for some common organic constituents are included in Appendix C. Although commonly specified as a constant value, this parameter can also be specified as a distribution of values. If constituent-specific data for the organic to be modeled are not available, this input value can be set to zero – a value that means the constituent's ground-water concentration will not be decreased due to adsorption.

Data Sources

Organic carbon partition coefficient (k_{oc}) values can be obtained from many constituent property handbooks, as well as online databases, (e.g., Kollig, Ellington, Karickhoff, Kitchens, Long, Weber and Wolfe, 1993 or *Handbook of Environmental Data on Organic Constituents*, Verschueren, 1983). Sometimes, these references provide an *octanol-water partition coefficient* (k_{ow}), rather than a k_{oc} value. These two coefficients are roughly equivalent parameters. A number of conversion formulas exist to convert k_{ow} values into k_{oc} ; these can be found in handbooks on environmental fate data (e.g., Verschueren, 1983; Kollig et. al., 1993). This conversion factor accounts for the mass difference, expressed as a percentage, between pure organic carbon and natural organic matter which also includes elements in addition to carbon (Enfield, Carsel, Cohen, Phan and Walters, 1982). Different conversion formulas exist for different constituents and environmental media, and there is no single formula that is valid for all organic constituents; therefore, the conversion formula should be chosen and used with some caution.

Use In EPACMTP

For organic constituents, the effect of equilibrium sorption is expressed in EPACMTP through the retardation coefficient, R , which is a function of the chemical-specific organic carbon partition coefficient, k_{oc} :

$$R = 1 + \frac{\rho_b k_d}{\theta} \quad (3.1)$$

where

$$k_d = f_{oc} \cdot k_{oc} \quad (3.2)$$

where

R	=	retardation coefficient for species i (dimensionless)
ρ_b	=	soil bulk density for the unsaturated zone (g/cm^3)
θ	=	soil water content (dimensionless)
k_d	=	soil-water partition coefficient (L/kg)
f_{oc}	=	fractional organic carbon content in the soil or aquifer (unitless)
k_{oc}	=	organic carbon partition coefficient (cm^3/g)

The fractional organic carbon can be estimated from the percentage organic matter (%OM) in the soil or aquifer, as

$$f_{oc} = \frac{\%OM}{174} \quad (3.3)$$

where

%OM = percent organic matter in the soil (unitless)
174 = conversion factor

3.3.2.2 Parameters Related to Chemical Hydrolysis

The transport of organic constituents can be influenced in part by chemical hydrolysis, a process that is represented in the EPACMTP model by means of an overall first-order chemical decay coefficient. This overall decay coefficient includes both dissolved phase and sorbed phase decay. Dissolved phase and sorbed phase decay rates can be specified directly, or they can be derived based on chemical-specific hydrolysis rate constants and the ground-water temperature and pH. In the latter case, the hydrolysis rate constants for each constituent can be obtained from reference documents compiled by EPA's Environmental Research Laboratory in Athens, GA (U.S. EPA, 1993 and Kollig et al., 1993).

The hydrolysis process as modeled in EPACMTP is affected by aquifer pH, aquifer temperature, and constituent sorption:

The overall first-order transformation rate for hydrolysis is calculated as:

$$\lambda = \frac{\lambda_1 \phi + \lambda_2 \rho_b k_d}{\phi + \rho_b k_d} \quad (3.4)$$

where:

λ	=	Overall first-order hydrolysis transformation rate (1/yr)
λ_1	=	Dissolved phase hydrolysis transformation rate (1/yr); see Section 3.3.2.2.1
λ_2	=	Sorbed phase hydrolysis transformation rate (1/yr); see Section 3.3.2.2.2
ϕ	=	Porosity (water content in the unsaturated zone) (dimensionless)
ρ_b	=	Bulk density (kg/L)
k_d	=	Partition coefficient (L/kg)

The calculation of the sorbed phase and dissolved phase hydrolysis rates from the hydrolysis rate constants is described in the following sections.

3.3.2.2.1 Dissolved Phase Hydrolysis Decay Rate (λ_1)

Definition

Hydrolysis is defined as the decomposition of organic constituents by interaction with water. The dissolved phase hydrolysis decay rate (1/yr) is the rate at which the dissolved portion of the contaminant mass is hydrolyzed.

Parameter Value or Distribution of Values

The dissolved phase hydrolysis decay rate can be directly input by the user (as either a constant value or distribution of values) or it can be set to be internally derived by the model. In the latter case, it is calculated as follows:

$$\lambda_1 = K_a^T [H^+] + K_n^T + K_b^T [OH^-] \quad (3.5)$$

where

$$\begin{aligned} \lambda_1 &= \text{First-order decay rate for dissolved phase (1/yr)} \\ K_a^T, K_n^T, K_b^T &= \text{Hydrolysis rate constants; calculated as described in Sections 3.3.2.2.3, 3.3.2.2.4, and 3.3.2.2.5} \\ [H^+] &= \text{Hydrogen ion concentration (mole/L)} \\ [OH^-] &= \text{Hydroxyl ion concentration (mole/L)} \end{aligned}$$

$[H^+]$ and $[OH^-]$ are computed from the pH of the soil or aquifer using

$$\begin{aligned} [H^+] &= 10^{-\text{pH}} \\ [OH^-] &= 10^{-(14-\text{pH})} \end{aligned}$$

Data Sources

In the absence of site-specific data, this parameter typically is set to be derived by the model based on the constituent-specific hydrolysis rate constants (see Sections 3.3.2.2.3 through 3.3.2.2.6).

Use In EPACMTP

The dissolved phase hydrolysis rate is used to calculate the overall first-order transformation rate for hydrolysis as presented in Equation 3.4.

3.3.2.2.2 Sorbed Phase Hydrolysis Decay Rate (λ_2)

Definition

Hydrolysis is defined as the decomposition of organic constituents by interaction with water. The sorbed phase hydrolysis decay rate (1/yr) is the rate at which the sorbed portion of the contaminant mass is hydrolyzed.

Parameter Value or Distribution of Values

The sorbed phase hydrolysis decay rate can be directly input by the user (as either a constant value or distribution of values) or it can be set to be internally derived by the model. If it is specified in the input file as derived by EPACMTP, the effective sorbed phase decay rate is calculated as:

$$\lambda_2 = 10K_a^T[H^+] + K_n^T \quad (3.6)$$

where:

λ_2	=	First-order hydrolysis rate for sorbed phase (1/yr)
K_a^T	=	Acid-catalyzed hydrolysis rate constant (1/mole/yr); see Section 3.3.2.2.3
K_n^T	=	Neutral hydrolysis rate constant (1/yr); see Section 3.3.2.2.4
10	=	Acid-catalyzed hydrolysis enhancement factor
$[H^+]$	=	Hydrogen ion concentration (computed from the pH of the soil or aquifer using $[H^+] = 10^{-\text{pH}}$)

Data Sources

In the absence of site-specific data, this parameter typically is set to be derived by the model based on the constituent-specific hydrolysis rate constants (see Sections 3.3.2.2.3 through 3.3.2.2.6).

Use In EPACMTP

The sorbed phase hydrolysis rate is used to calculate the overall first-order transformation rate for hydrolysis as presented in Equation 3.4.

3.3.2.2.3 Acid-Catalyzed Hydrolysis Rate Constant (K_a^{Tr})

Definition

The tendency of a constituent to hydrolyze is expressed through several constituent-specific rate constants. The acid-catalyzed rate constant (1/mol-yr) is one of the values that is used to quantify how the rate of the hydrolysis reaction is affected

by the pH (specifically at the acidic end of pH) of the subsurface. The superscript T_r indicates that the value is measured at a specified reference temperature.

Parameter Value or Distribution of Values

The acid-catalyzed rate constant is a constituent-specific input parameter; values for some common organic constituents are included in Appendix C. Although commonly specified as a constant value, this parameter can also be specified as a distribution of values. If constituent-specific data for the organic to be modeled are not available, this input value can be set to zero – a conservative value that means the constituent's ground-water concentration will not be decreased due to chemical hydrolysis at the acidic end of the scale. However, if the modeled constituent hydrolyzes to form one or more toxic degradation products, then setting this input to zero and not modeling the formation of the toxic degradation product could result in an underestimation of the risk of exposure via the ground-water pathway.

Data Sources

$(K_a^{T_r})$ values can be obtained from some constituent property handbooks (e.g., Kollig et al, 1993 or *Handbook of Environmental Data on Organic Constituents*, Verschueren, 1983).

Use In EPACMTP

The acid-catalyzed hydrolysis rate constant is influenced by ground-water temperature, while acid- and base catalyzed rate constants are also influenced by pH. As shown below, the Arrhenius equation is used to convert the input hydrolysis rate constants, measured at a specified reference temperature (T_r), to the actual temperature of the subsurface:

$$K_J^T = K_J^{T_r} \exp [E_a/R_g(\frac{1}{T_r + 273} - \frac{1}{T + 273})] \quad (3.7)$$

K_J^T	=	Hydrolysis rate constant for reaction process J, corrected for the subsurface temperature T_r (1/mol-yr for the acid- and base-catalyzed reactions; 1/yr for the neutral reaction)
$K_J^{T_r}$	=	Hydrolysis rate constant for reaction process J, measured at reference temperature T (1/mol-yr for the acid- and base-catalyzed reactions; 1/yr for the neutral reaction)
J	=	a for the acid-catalyzed reaction, b for base-catalyzed reaction, and n for the neutral reaction
T	=	Temperature of the subsurface (°C)
T_r	=	Reference temperature (°C)
R_g	=	Universal gas constant (1.987E-3 Kcal/deg-mole)
E_a	=	Arrhenius activation energy (Kcal/mole)

Note that, using the generic activation energy of 20 Kcal/mole recommended by Wolfe (1985), the factor E_a/R_g has a numerical value of 10,000.

The temperature-corrected rate constants are then used in Equations 3.5 and 3.6 to calculate the sorbed phase and dissolved phase hydrolysis rate constants from which the overall hydrolysis transformation rate is calculated. The overall first-order transformation rate is one of the parameters required to solve the advection-dispersion equation (see Sections 3.3.4 and 4.4.4 of the *EPACMTP Technical Background Document* (U.S. EPA, 2003a)).

3.3.2.2.4 Neutral Hydrolysis Rate Constant (K_n^{Tr})

Definition

The tendency of a constituent to hydrolyze is expressed through several constituent-specific rate constants. The neutral rate constant (1/yr) is used to quantify how the rate of the hydrolysis reaction is unaffected by the pH of the subsurface. The superscript T_r indicates that the value is measured at a specified reference temperature.

Parameter Value or Distribution of Values

The neutral rate constant is a constituent-specific input parameter; values for some common organic constituents are included in Appendix C. Although commonly specified as a constant value, this parameter can also be specified as a distribution of values. If constituent-specific data for the organic to be modeled are not available, this input value can be set to zero – a conservative value that means the constituent's ground-water concentration (under pH neutral conditions) will not be decreased due to chemical hydrolysis. However, if the modeled constituent hydrolyzes to form one or more toxic degradation products, then setting this input to zero and not modeling the formation of the toxic degradation product could result in an underestimation of the risk of exposure via the ground-water pathway.

Data Sources

K_n^{Tr} values can be obtained from some constituent property handbooks (e.g., Kollig et al, 1993 or *Handbook of Environmental Data on Organic Constituents*, Verschueren, 1983).

Use In EPACMTP

As shown in Equation 3.7, the Arrhenius equation is to used convert the input hydrolysis rate constants, measured at a specified reference temperature (T_r), to the actual temperature of the subsurface. The temperature-corrected rate constants are then used in Equations 3.5 and 3.6 to calculate the sorbed phase and dissolved phase hydrolysis rate constants from which the overall hydrolysis transformation rate is calculated. The overall first-order transformation rate is one of the parameters required to solve the advection- dispersion equation (see Sections 3.3.4 and 4.4.4 of the *EPACMTP Technical Background Document* (U.S. EPA, 2003a)).

3.3.2.2.5 Base-Catalyzed Hydrolysis Rate Constant (K_b^{Tr})

Definition

The tendency of each constituent to hydrolyze is expressed through several constituent-specific rate constants. The base-catalyzed rate constant (1/mol-yr) is one of the values that is used to quantify how the rate of the hydrolysis reaction is affected by the pH of the subsurface, in this case under more alkaline conditions. The superscript T_r indicates that the value is measured at a specified reference temperature.

Parameter Value or Distribution of Values

The base-catalyzed rate constant is a constituent-specific input parameter; values for some common organic constituents are included in Appendix C. Although commonly specified as a constant value, this parameter can also be specified as a distribution of values. If constituent-specific data for the organic to be modeled are not available, this input value can be set to zero – a conservative value that means the constituent's ground-water concentration will not be decreased due to chemical hydrolysis at the alkaline end of the scale. However, if the modeled constituent hydrolyzes to form one or more toxic degradation products, then setting this input to zero and not modeling the formation of the toxic degradation product could result in an underestimation of the risk of exposure via the ground-water pathway.

Data Sources

The K_b^{Tr} values can be obtained from some constituent property handbooks (e.g., Kollig et al, 1993 or *Handbook of Environmental Data on Organic Constituents*, Verschueren, 1983).

Use In EPACMTP

As shown in Equation 3.7, the Arrhenius equation is used to convert the input hydrolysis rate constants, measured at a specified reference temperature (T_r), to the actual temperature of the subsurface. The temperature-corrected rate constants are then used in Equations 3.5 and 3.6 to calculate the sorbed phase and dissolved phase hydrolysis rate constants from which the overall hydrolysis transformation rate is calculated. The overall first-order transformation rate is one of the parameters required to solve the advection-dispersion equation (see Sections 3.3.4 and 4.4.4 of the *EPACMTP Technical Background Document* (U.S. EPA, 2003a)).

3.3.2.2.6 Reference Temperature (T_r)

Definition

The reference temperature ($^{\circ}\text{C}$) is the temperature at which the input hydrolysis rate constants were measured.

Parameter Value or Distribution of Values

The chemical-specific hydrolysis rate constants are measured at a constant reference temperature; the default value is 25 degrees Celsius.

Data Sources

Hydrolysis rate constants can be obtained from some constituent property handbooks (e.g., Kollig et al, 1993 or *Handbook of Environmental Data on Organic Constituents*, Verschueren, 1983). The data source used for the hydrolysis rate constants should also state the temperature at which the values were measured.

Use In EPACMTP

As shown in Equation 3.7, the reference temperature is used in the Arrhenius equation to convert the input hydrolysis rate constants to the actual temperature of the subsurface. The temperature-corrected rate constants are then used in Equations 3.5 and 3.6 to calculate the sorbed phase and dissolved phase hydrolysis rate constants from which the overall hydrolysis transformation rate is calculated. The overall first-order transformation rate is one of the parameters required to solve the advection-dispersion equation (see Sections 3.3.4 and 4.4.4 of the *EPACMTP Technical Background Document* (U.S. EPA, 2003a)).

3.3.2.3 Parameters Related to Hydrolysis Transformation Products

In the event that the products of this chemical degradation process are toxic and their constituent-specific parameters are known, they can be included in the simulation by specifying them to be part of a transformation (or decay) chain. Note that when a multi-species simulation such as this is performed, the necessary chemical-specific parameters must be repeated for each species in the decay chain. In addition, the following parameters are required for each degradation species in a decay chain analysis: degradation product species number, number of immediate parents for each degradation product species, species number(s) of immediate parent(s), and fraction of the parent species that decays into the given degradation product species.

3.3.2.3.1 Degradation Product Species Number (I)**Definition**

The degradation product species number is an index number that uniquely identifies a constituent and its properties in EPACMTP.

Parameter Value or Distribution of Values

Degradation product species numbers begin with the number 2 (the parent species number is 1). Up to 6 degradation products per parent are permitted in EPACMTP (numbered 2-7).

Data Sources

The degradation product species number is a construction of convenience for EPACMTP, and as such, there are no data sources. The value of the parameter is governed by the number of degradation products in a particular transformation chain.

Use In EPACMTP

The degradation product species number allows EPACMTP to track and associate degradation products with its properties and relationships to its immediate parent and daughters.

3.3.2.3.2 Number of Immediate Parents (M_i)**Definition**

The number of immediate parents (M_i) is defined as the total number of individual species which degrade directly into degradation product species ℓ . This parameter is used in EPACMTP together with the species number of the immediate parent (see next section) to represent the structure of the chain decay reaction. The value of this parameter is zero for the parent species and one for each degradation product species. The maximum value of M_i is one because the EPACMTP model can handle simulation of only one constituent that has a non-zero initial leachate concentration (that is, one original parent species per decay chain). For example, if constituent A degrades into constituent B, and B degrades to C, then degradation product B has one immediate parent (A) and degradation product C also has one immediate parent (B).

Parameter Value or Distribution of Values

The number of immediate parent species is governed by the specific transformation chain to be simulated using EPACMTP.

Data Sources

The number of immediate parent species is governed by the decay chain reaction being simulated. Reaction chemistry or constituent property handbooks (e.g., Kollig et al, 1993, or Handbook of Environmental Data on Organic Constituents, Verschueren, 1983) may contain chain decay structures for organic constituents.

Use In EPACMTP

The number of immediate parent species of a degradation product species allows EPACMTP to track its relationships to its immediate parent.

3.3.2.3.3 Species Number(s) of Immediate Parent(s) ($m_{\ell}(i)$, $i = 1, M_{\ell}$)

Definition

The species number $m_{\ell}(i)$ of the immediate parent is the ordinal number (see Section 3.3.2.3.1) of the toxic degradation product that directly degrades into the degradation product of concern. For example, consider again the straight decay chain where constituent A degrades into constituent B which degrades into constituent C shown in the example below:

Parameter	Definition	Value for Constituent A	Value for Constituent B	Value for Constituent C
ℓ	species number	1	2	3
M_{ℓ}	number (quantity) of immediate parents	0	1	1
$m_{\ell}(i)$	species number of immediate parent	0	1	2

Parameter Value or Distribution of Values

The species number of immediate parent species is governed by the specific decay chain to be simulated using EPACMTP and by the numbering system chosen by the user.

Data Sources

The numbering of immediate parent species is governed by the decay chain reaction being simulated and the user's discretion. Reaction chemistry or constituent property handbooks (e.g., Kollig et al, 1993, or *Handbook of Environmental Data on Organic Constituents*, Verschueren, 1983) may contain chain decay structures for organic constituents.

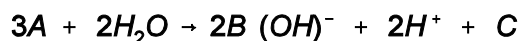
Use In EPACMTP

The association of an immediate parent to a degradation product species number allows EPACMTP to track and associate a degradation product with its properties and relationships to its immediate parent and degradation products.

3.3.2.3.4 Fraction of the Parent Species (ξ_{lm})

Definition

The coefficient ξ_{lm} is called the fraction of the parent species which expresses how many units of species l are produced in the decay of each unit of parent m . The value of the speciation factor is thus determined by the reaction stoichiometry, as well as the units used to express concentration. For instance, consider the following hydrolysis reaction in which 2 units of degradation product B and 1 unit of degradation product C are formed from the hydrolysis of 3 units of parent A:



where

A	=	parent compound A
H ₂ O	=	water molecule
B	=	degradation product compound B
C	=	degradation product compound C
(OH) ⁻	=	hydroxide ion
H ⁺	=	hydrogen ion

In this example, ξ_{BA} is equal to $\frac{2}{3} \frac{MW_B}{MW_A}$ and ξ_{CA} is equal to $\frac{1}{3} \frac{MW_C}{MW_A}$

where

MW_ℓ	=	the molecular weight of species ℓ (g/mol)
ξ_{BA}	=	speciation factor between parent A and degradation product B
ξ_{CA}	=	speciation factor between parent A and degradation product C

Parameter Value or Distribution of Values

The value of this parameter is determined by the species and reaction stoichiometry and is constant for the entire simulation.

Data Sources

The fraction of parent species is governed by the stoichiometry of the decay chain reaction being simulated and individual constituent properties. Reaction chemistry or constituent property handbooks (e.g., Kollig et al, 1993, or *Handbook of Environmental Data on Organic Constituents*, Verschueren, 1983) may contain chain decay structures for organic constituents.

Use In EPACMTP

EPACMTP uses the fraction of parent species to determine how much of a parent species decays to form an immediate daughter. Similarly, the same factor is used to determine how much degradation product species is produced from its immediate parent. These relationships are applied in both the unsaturated and saturated fate and transports simulations (see Equations 3.14 and 4.31, respectively in the *EPACMTP Technical Background Document*, (U.S. EPA, 2003a)).

3.3.3 Metals

In the subsurface, metal constituents may undergo reactions with ligands in the pore water and with surface sites on the solid aquifer or soil matrix material. Reactions in which the metal is bound to the solid matrix are referred to as sorption reactions and metal that is bound to the solid is said to be sorbed. The ratio of the concentration of metal sorbed to the concentration in the mobile aqueous phase at equilibrium is referred to as the partition coefficient (K_d). During contaminant transport, sorption to the solid matrix results in retardation of the contaminant front. Thus, transport models such as EPACMTP incorporate the contaminant partition coefficient into the overall retardation factor (the ratio of the average linear particle velocity to the velocity of that portion of the plume where the contaminant is at 50 percent dilution). The use of K_d in EPACMTP transport modeling implies the assumption that local equilibrium between the solutes and the sorbents is attained, meaning that the rate of sorption reactions is fast relative to advective-dispersive transport of the contaminant.

Users can specify a constant value or distribution of values for the K_d (a linear isotherm); alternatively, tables of non-linear sorption isotherms (for a suite of 21 metals, some with varying oxidation states) or equations comprising pH-based (linear) isotherms are available within EPACMTP. Both the non-linear isotherms and the pH-based isotherms were developed especially for use with the EPACMTP model.

The pH-dependent isotherms were developed for 12 metals using the empirical relationships as described in Loux, Chafin and Hassan (1990). These isotherms were originally developed as an alternative to the MINTEQA2-derived isotherms (U.S. EPA, 1996 and 1999) because, at that time, there were limitations in the database of adsorption reactions that made the MINTEQA2 modeling less accurate for metals that form anions or neutral species in aqueous solution. However, ensuing improvements in the MINTEQA2 database of adsorption reactions and modeling methodology have resulted in a new set of non-linear isotherms which supercede the pH-based isotherms. However, the option to use these pH-based isotherms is still available in the EPACMTP model, and so they are described in this document.

The non-linear isotherms were estimated using the geochemical speciation model, MINTEQA2, and are tabulated into auxiliary input files for use by the EPACMTP model. These isotherms reflect the tendency of K_d to decrease as the total metal concentration in the system increases. The non-linear isotherms available for use in EPACMTP are specified in terms of the dissolved metal concentration and the corresponding sorbed concentration at a series of total metal concentrations.

For a particular metal, K_d values in a soil or aquifer are dependent upon the metal concentration and various geochemical characteristics of the soil or aquifer and the associated pore water. Geochemical parameters that have the greatest influence on the magnitude of K_d include the pH of the system and the nature and concentration of sorbents associated with the soil or aquifer matrix. In the subsurface beneath a disposal facility, the concentration of leachate constituents may also influence K_d . Although the dependence of metal partitioning on the total metal concentration and on pH and other geochemical characteristics is apparent from partitioning studies reported in the scientific literature, K_d values for many metals are not available for the range of metal concentrations or geochemical conditions needed in risk assessment modeling. For this reason, MINTEQA2 was used to estimate partition coefficients. The use of a speciation model allows K_d values to be estimated for a range of total metal concentrations in various model systems designed to depict natural variability in those geochemical characteristics that most influence metal partitioning.

The development of these non-linear (concentration-dependent) metal partition coefficients is described in Appendix B.1. The following sections describe the available options and the input parameters required to perform ground-water fate and transport modeling of metal constituents using the EPACMTP model.

3.3.3.1 Empirical K_d Data

There are two sources of empirical K_d data that can be used to model metals transport using linear isotherms: K_d data compiled from a recent comprehensive literature survey and pH-based isotherms that are based on the empirical laboratory-based data of Loux et al (1990). These two types of empirical K_d data are described in the following sections.

3.3.3.1.1 K_d Data Compiled from a Literature Survey

In the absence of site-specific data, the distribution coefficient for metals can be specified as a statistical or empirical distribution of values. A comprehensive literature review of K_d values was conducted for the EPA's *RCRA Hazardous Waste Listing Determination for Inorganic Chemical Manufacturing Wastes* (U.S. EPA, 2000). For this project, K_d was defined as an empirical distribution of values when sufficient data were available (six or more literature K_d values) or as a log uniform distribution of values when fewer data were found in the scientific literature (five or fewer literature K_d values). This literature review focused on identifying and compiling experimentally derived K_d values for soil and aquifer materials from published literature. Collected values were compiled along with geochemical and measurement parameters most likely to influence K_d . Details of the literature search and data collection strategy are given in Appendix I of the *Risk Assessment for the Listing Determination for Inorganic Chemical Manufacturing Wastes: Background Document* (U.S. EPA, 2000) along with the resulting distributions of K_d values.

If site-specific K_d data are unavailable, the EPACMTP user can specify that one of these default distributions be used for the coefficient of the Freundlich isotherm for the unsaturated and saturated zones. That is, the appropriate distribution, gleaned

from (U.S. EPA, 2000), should be entered twice in the EPACMTP input file, once in the unsaturated zone parameter group and again for the aquifer parameter group.

3.3.3.1.2 pH-based Isotherms

pH-dependent isotherms for 15 metal species were determined from empirical relationships as described in Loux et al., 1990. Many of these metals form anions or neutral species in aqueous solution (e.g., HAsO_3^{2-} , H_2AsO_3^- , and H_3AsO_3^0).

The pH-dependent empirical relationships were determined from linear least squares analysis of laboratory measurements from aquifer materials and their corresponding ground water and leachate samples collected from six municipal landfills, as well as other published data. In these experiments, the concentrations of trace metal contaminants in the ground-water/aquifer material samples were augmented with additions (spikes), and the spiked samples were allowed to equilibrate for 48 hours. After equilibration, the trace metal remaining in solution was measured. The difference between the total trace metal in the system (the metal originally in the sample plus the amount added) and the amount remaining in solution at equilibrium was regarded as adsorbed. The distribution coefficient was determined as the ratio of amount of trace metal adsorbed to the amount remaining in solution. The resulting relationships give K_d as a function of pH only; the inherent nonlinear character of metal adsorption as a function of total metal concentration is not represented.

In EPACMTP Monte Carlo analyses for nationwide assessments, a different pH value is generated for each Monte Carlo iteration. Upon the selection of a pH, the corresponding K_d is automatically calculated from the appropriate empirical relationship.

No empirical relation was available for Sb^{III} ; so the Sb^{V} relationship can be used for both the +3 and +5 oxidation states. Also, the As^{III} species is adsorbed somewhat less strongly than As^{V} , and Se^{VI} is adsorbed less strongly than Se^{IV} . However, the contrast in adsorption affinity between different oxidation states for these metals is not nearly so marked as the contrast in Cr^{III} and Cr^{VI} . Therefore, the As^{III} and Se^{VI} relationships can be used to represent both oxidation states for these metals. The resulting empirical relationships are presented in Table 3.3.

Table 3.3 Empirical pH-dependent Adsorption Relations (Loux et al., 1990)

Metal Species	K_d (liters kg^{-1})
As ^{III}	10 (0.0322 pH + 1.24)
Ba ^{II}	10 (0.190 pH + 0.638)
Cd ^{II}	10 (0.397 pH - 0.943)
Cr ^{VI}	10 (-0.117 pH + 2.07)
Hg ^{II}	10 (0.122 pH + 1.42)
Ni ^{II}	10 (0.332 pH - 0.471)
Pb ^{II}	10 (0.0768 pH + 1.55)
Sb ^V	10 (-0.207 pH + 2.996)
Se ^{VI}	10 (-0.296 pH + 2.71)
Tl	10 (0.110 pH + 1.102)

3.3.3.2 MINTEQA2-Derived Sorption Isotherm Data

In the absence of site-specific data, the distribution coefficient for metals can be automatically drawn from tabulated data comprising a set of non-linear sorption isotherms created especially for use with the EPACMTP model. This option for modeling the fate and transport of selected metals incorporates metal-specific geochemical interactions that control the mobility of metals in the subsurface. This modeling procedure was originally developed at the EPA's National Exposure Research Laboratory, Ecosystems Research Division for the Hazardous Waste Identification Rule (HWIR) and utilizes nationwide distributions of key geochemical parameters that impact metal mobility in the subsurface.

In this methodology, the MINTEQA2 metal speciation code was used to generate nonlinear adsorption isotherms for each metal. That is, a set of isotherms was produced for each metal reflecting the range in geochemical environments expected at waste sites across the nation.

To compute the adsorption distribution coefficient (K_d) values for a particular metal, a value was selected for each of the five master variables and the MINTEQA2 model was executed over a range of total metal concentrations. The result is a nonlinear adsorption isotherm that can be represented by the variation in K_d with total metal concentration (or, with equilibrium dissolved concentration). This procedure was repeated (separately for each metal) for numerous combinations of master variable settings. The final result from MINTEQA2 was nonlinear K_d versus metal concentration curves for combinations of master variable settings spanning the range of reasonable values.

For each metal, the resulting set of isotherms was tabulated into a supplementary input data file for use by the EPACMTP model. In the fate and transport modeling for a particular metal, EPACMTP is executed and the probability distributions for these five variables form the basis for the Monte-Carlo selection of the appropriate

adsorption isotherm. A detailed discussion of the MINTEQA2 simulation procedure for generating the metals sorption isotherms is provided in Appendix B.1.

MINTEQA2-derived sorption isotherms have been developed for the following metals: antimony (V), arsenic (III), barium, beryllium, cadmium, chromium (III), chromium (VI), copper (II), mercury (II), nickel, lead, selenium (VI), thallium (I), vanadium, and zinc.

As implemented in EPACMTP, it is assumed that the non-linearity of the isotherms is most important in the unsaturated zone where metals concentrations are relatively high. Although MINTEQA2 isotherms were also generated for the saturated zone, upon reaching the water table and mixing of the leachate with ambient ground water, the metals concentration is considered to be low enough that a linear isotherm (single K_d value not dependent on metal concentration) can always be used. The appropriate saturated zone retardation factor is determined based on the maximum ground-water concentration underneath the source.

Geochemical factors that are known to have direct impact on adsorption in ground-water systems are: (1) ground-water composition, (2) subsurface pH, (3) hydrous ferric oxide adsorbent content of the soil/aquifer in the subsurface, (4) concentration of organic acids in the leachate, and (5) natural soil organic matter content of the soil/aquifer in the subsurface (particulate and dissolved). For a given metal at a given total concentration, the propensity for adsorption changes greatly as these parameters vary. For the MINTEQA2 modeling, two ground-water types were used (carbonate and non-carbonate) and for each ground-water type, the natural variability of the remaining three parameters (since only low concentrations of leachate organic acids are expected in the leachate emanating from industrial waste management units, only the low range was modeled for leachate organic acid content) was divided into three ranges: high, medium, and low. The approximate mid-point of each range was identified, and in the MINTEQA2 modeling, these mid-point values were used to simulate each range of values for pH, hydrous ferric oxide content, and natural organic matter. For the non-carbonate ground-water type, one isotherm (as a function of metal concentration) was developed for each combination of the three possible values for the four master variables. This process was then repeated for the carbonate ground-water type. For each ground-water type, separate isotherms were developed for the unsaturated and saturated zone. For each metal, a set of 648 isotherms was developed.

The following EPACMTP input parameters are required to model metals transport using the MINTEQA2 non-linear isotherms: metal identification number, soil and aquifer pH, hydrous ferric oxide adsorbent content, leachate organic matter concentration, percent organic matter of the soil, fraction organic carbon of the aquifer, and ground-water composition. Each of these inputs, including the data sources and the default EPACMTP input distributions (which correspond to the values used in the MINTEQA2 modeling) for each of the five master variables, are described in the following sections.

3.3.3.2.1 Metal Identification Number (ID)***Definition***

The metal identification number is simply an arbitrary number assigned to each metal in order to provide a simple means of specifying which metal is being modeled.

Parameter Value or Distribution of Values

The metal contaminants whose partition coefficients have been estimated using MINTEQA2 include arsenic (As), antimony (Sb), barium (Ba), beryllium (Be), cadmium (Cd), cobalt (Co), copper (Cu), chromium (Cr), fluoride (F), mercury (Hg), manganese (Mn), molybdenum (Mo), lead (Pb), nickel (Ni), selenium (Se), silver (Ag), thallium (Tl), vanadium (V), and zinc (Zn).

Several of these metals occur naturally in more than one oxidation state. The modeling described here is restricted to the oxidation states that are most likely to occur in waste systems or most likely to be mobile in ground-water waste systems. For arsenic, chromium, and selenium, partition coefficients were estimated for two oxidation states. These were: As(III) and As(V), Cr(III) and Cr(VI), and Se(IV) and Se(VI). For antimony, molybdenum, thallium, and vanadium, only one oxidation state was modeled although multiple oxidation states occur. For all four of these metals, the choice of which state to model was dictated by practical aspects such as availability of sorption reactions and by subjective assessment of the appropriate oxidation state. The oxidation states modeled were Sb(V) (there were no sorption reactions available for Sb(III)), Mo(VI) (molybdate seems the most relevant form from literature reports), thallium (I) (this form is more frequently cited in the literature as having environmental implications), and V(V) (vanadate; sorption reactions were not available for other forms).

The metal identification number for each metal with a set of MINTEQA2-derived non-linear isotherms is presented in Table 3.4. The appropriate identification number should be specified in the EPACMTP input file as a constant value.

Table 3.4 Metals that have MINTEQA2-derived Non-linear Isotherms

Metal Species	Metal ID
Ba	1
Cd	2
Cr (III)	3
Hg	4
Ni	5
Pb	6
Ag	7
Zn	8
Cu	9
V	10
Be	11
Mo	12
As (III)	13
Cr (VI)	14
Se (VI)	15
Tl	16
Sb (V)	17
Co	18
Mn	19
F	20
As (V)	21
Se (IV)	22

Data Sources

These metal identification numbers were arbitrarily created for convenience during modeling; the list of available metals was determined by the availability of toxicity and sorption data and their likely occurrence in industrial waste management scenarios under consideration for Agency rule-making.

Use In EPACMTP

The metal identification number is used by the EPACMTP model to identify which supplemental input file contains the appropriate non-linear isotherm data.

3.3.3.2.2 Soil and Aquifer pH (pH)

Definition

A measure of the acidity or alkalinity of the moisture present in the vadose zone or the ground water. pH is measured on a scale of 0 to 14, with 7 representing a neutral state. Values less than 7 are acidic, and values greater than 7 are basic. pH is calculated as the negative logarithm of the concentration of hydrogen ions in a solution.

For modeling purposes, pH is assumed to be the same in the unsaturated zone and in the saturated zone.

Parameter Value or Distribution of Values

Lacking a site-specific value or distribution of values, a default distribution of pH values may be used. The data are represented by an empirical distribution with low and high values of 3.2 and 9.7, respectively and a median value of 6.8. The distribution is shown in Figure 3.5.

Table 3.5 Probability distribution of soil and aquifer pH

Cumulative Probability (%)	pH Value
0.0	3.21E+00
1.0	5.40E+00
5.0	6.31E+00
10.0	7.11E+00
25.0	7.59E+00
50.0	7.69E+00
75.0	7.80E+00
90.0	7.90E+00
95.0	8.09E+00
100.0	9.69E+00

Data Sources

The distribution of pH values shown in Table 3.5 was obtained through analysis of nearly 25,000 field measured pH values of uncontaminated ground water obtained from EPA's STORET database (U.S. EPA, 1996). Note that the upper and lower bounds of this distribution were established by reference to reported values in the open literature.

Use In EPACMTP

The ground-water pH is one of the most important subsurface parameters controlling the mobility of metals. Most metals are more mobile under acidic (low pH) conditions, as compared to neutral or alkaline (pH of 7 or higher) conditions. The pH may also affect the hydrolysis rate of organic constituents; some constituents degrade

more rapidly or more slowly as pH varies. The pH of most aquifer systems is slightly acidic, the primary exception being aquifers in solution limestone settings. These may also be referred to as 'karst', 'carbonate' or 'dolomite' aquifers. The ground water in these systems is usually alkaline.

The EPACMTP model assumes that the ground-water/aquifer system is well buffered with respect to pH. That is, in the modeling analysis, there is no effect on the ambient pH from the leachate emanating from the base of the WMU.

3.3.3.2.3 Iron Hydroxide Content (FeOx)

Definition

The nature and amount of solid matter in the subsurface to which metals are attracted (the adsorbent) are important in determining the extent to which a constituent's transport through the ground-water pathway is retarded due to adsorption. Iron hydroxides (FeOx) represent one of the dominant adsorbents for metal sorption in environmental systems, and were one of the geochemical master variables used in the calculation of the non-linear sorption isotherms using the MINTEQA2 model. Although other sorbents such as clay minerals, carbonate minerals, hydrous aluminum and manganese oxides, and silica may sorb metals in the subsurface, accounting for ferric hydroxide and particulate organic matter (see Section 3.3.3.2.5 for a discussion on particulate organic matter) is sufficient to produce a realistic, yet protective, modeling analysis for most natural ground-water systems.

Parameter Value or Distribution of Values

In the MINTEQA2 modeling that was used to calculate the isotherms for a number of metals, the type of ferric oxide that was assumed to be present was in the form of the mineral goethite (FeOOH), a common form of ferric oxide in soils. A database of sorption reactions for goethite reported by Mathur (1995) was used with the diffuse-layer sorption model in MINTEQA2 to represent the interactions of protons and metals with the goethite surface. Further details of the MINTEQA2 modeling procedure are given in Appendix B.1.

Lacking a site-specific value or distribution of values for this input parameter, a default distribution may be used. The limited data on iron hydroxide content that are available (Loux et al., 1990) were used to define a uniform distribution, with a minimum of 0.0126 and a maximum of 1.115 percent iron hydroxide by weight. A summary of this default distribution is presented in Table 3.6.

Table 3.6 Probability distribution of fraction iron hydroxide

Cumulative Probability (%)	Iron Hydroxide Content (wt %)
0.0	1.82E-02
1.0	2.89E-02
5.0	4.37E-02
10.0	6.85E-02
25.0	9.36E-02
50.0	9.84E-02
75.0	1.04E-01
90.0	1.09E-01
95.0	1.14E-01
100.0	1.19E-01

Data Sources

The default distribution is based on analyses by Loux et al., (1990) on aquifer samples collected by the U.S. EPA Office of Solid Waste (OSW) in Florida, New Jersey, Oregon, Texas, Utah, and Wisconsin.

Use In EPACMTP

The iron hydroxide content of the subsurface is one of the most important subsurface parameters controlling the mobility of metals. In EPACMTP, accounting for ferric hydroxide determines the extent to which a constituent's transport through the ground-water pathway is retarded due to adsorption.

3.3.3.2.4 Leachate Organic Matter (LOM)**Definition**

In addition to the metal contaminants, the leachate exiting a WMU may contain elevated concentrations of leachate organic matter. This organic matter may consist of various compounds including organic acids that represent primary disposed waste or that result from the breakdown of more complex organic substances. Many organic acids found in leachate have significant metal-complexing capacity that may influence metal mobility. This input represents the concentration of these anthropogenic organic acids in the leachate emanating from the base of the WMU.

Parameter Value or Distribution of Values

Lacking a site-specific value or distribution of values for the concentration of organic acids in the leachate (which can then be used to help generate site-specific k_d values), the influence of leachate organic matter on metal sorption may be represented by using a default distribution of values for this input parameter. The default distribution is uniform, with a minimum of 0.001173 mg/L and a maximum of 0.00878 mg/L. A summary of this default distribution is presented in Table 3.7.

Table 3.7 Probability distribution of leachate organic matter

Cumulative Probability (%)	Concentration of Leachate Organic Matter (mg/L)
0.0	1.05E+02
1.0	1.40E+02
5.0	1.94E+02
10.0	2.84E+02
25.0	3.76E+02
50.0	3.94E+02
75.0	4.12E+02
90.0	4.30E+02
95.0	4.47E+02
100.0	4.67E+02

Data Sources

In an effort to incorporate in the ground-water modeling the solubilizing effect of organic acids, a default distribution of leachate organic matter concentrations was developed based on data presented by Gintautas, Huyck, Daniel, and Macalady (1993). This study examined leachates from six landfills from across the U. S. and found that over 30 different acids were present. The range of leachate organic matter concentration levels given in the default distribution is based on the measured total organic carbon among the six landfill leachates in this study.

Use In EPACMTP

The concentration of anthropogenic organic acids in leachate is one of the most important subsurface parameters controlling the mobility of metals. In EPACMTP, this parameter is used to quantify metal-complexing capacity that may influence metal mobility.

3.3.3.2.5 Percent Organic Matter (%OM)***Definition***

The nature and amount of solid matter in the subsurface to which metals are attracted (the adsorbent) are important in determining the extent to which a constituent's transport through the ground-water pathway is retarded due to adsorption. Particulate organic matter present in the unsaturated zone (input to EPACMTP as percent organic matter) represents one of the dominant adsorbents for metal sorption in environmental systems and was one of the geochemical master variables used in the calculation of the non-linear sorption isotherms using the MINTEQA2 model. Although other sorbents such as clay minerals, carbonate minerals, hydrous aluminum and manganese oxides, and silica may sorb metals in the subsurface, accounting for ferric hydroxides (See Section 3.3.3.2.3 for a discussion of FeOx) and particulate organic matter (in the soil and aquifer) is sufficient to produce a realistic, yet protective, modeling analysis for most natural ground-water systems. In EPACMTP modeling, the

amount of particulate organic matter in the soil (as opposed to the aquifer, represented by the term f_{oc}) is represented by the percent organic matter (%OM).

Parameter Value or Distribution of Values

Lacking a site-specific value or distribution of values for this input parameter (which can then be used to help generate site-specific k_d values), a default distribution may be used. In the EPACMTP model, there are three default soil types (sandy loam, silty loam, and silty clay loam); each soil type has a unique distribution of values for each of the soil parameters, including the percent organic matter. When modeling a metal using the MINTEQA2-derived isotherms, the default distribution for percent organic matter in the unsaturated zone is based on the default distribution for percent organic matter for the silty loam soil type. The silty loam soil type is intermediate in weight percent organic matter in comparison with the other two and is the most frequently occurring soil type. The default distribution type is Johnson SB; the minimum value is 0.0 and the maximum value is 8.51. A summary of this default distribution is presented in Table 3.8.

Table 3.8 Probability distribution of percent organic matter in the unsaturated zone

Cumulative Probability (%)	Percent Organic Matter in the Unsaturated Zone (unitless)
0.0	4.08E-03
1.0	3.76E-02
5.0	6.07E-02
10.0	1.04E-01
25.0	1.78E-01
50.0	2.04E-01
75.0	2.38E-01
90.0	2.87E-01
95.0	3.82E-01
100.0	1.80E+00

Data Sources

The default distribution described above for the percent organic matter in the unsaturated zone is based on data presented in Carsel and Parrish, 1988.

Use In EPACMTP

The percent organic matter in the unsaturated zone is used in EPACMTP because the nature and amount of solid matter in the subsurface to which metals are attracted (the adsorbent) are important in determining the extent to which a constituent's transport through the ground-water pathway is retarded due to adsorption. As the adsorption of a contaminant in the unsaturated zone increases, more of the contaminant is removed from the system, and is unavailable for transport.

3.3.3.2.6 Fraction Organic Carbon (f_{oc})**Definition**

The nature and amount of solid matter in the subsurface to which metals are attracted (the adsorbent) are important in determining the extent to which a constituent's transport through the ground-water pathway is retarded due to adsorption. Particulate organic matter present in the saturated zone represents one of the dominant adsorbents for metal sorption in environmental systems and was one of the geochemical master variables used in the calculation of the non-linear sorption isotherms using the MINTEQA2 model. Although other sorbents such as clay minerals, carbonate minerals, hydrous aluminum and manganese oxides, and silica may sorb metals in the subsurface, accounting for ferric hydroxide (see Section 3.3.3.2.3 for a discussion of FeOx) and particulate organic matter (in the soil and aquifer) is sufficient to produce a realistic, yet protective, modeling analysis for most natural ground-water systems. In EPACMTP modeling, the amount of particulate organic matter in the aquifer is represented by the fraction organic carbon, or f_{oc} (as opposed to the soil, represented by the term %OM).

Parameter Value or Distribution of Values

Lacking a site-specific value or distribution of values for this input parameter (which can then be used to help generate site-specific k_d values), a default distribution may be used. In the EPACMTP model, there are three default soil types (sandy loam, silty loam, and silty clay loam); each soil type has unique distribution of values for each of the soil parameters, including the percent organic matter. When modeling a metal using the MINTEQA2-derived isotherms, the default distribution for fraction organic carbon in the saturated zone is based on the default distribution for percent organic matter for the sandy loam soil type, however, this value is converted from percent organic matter to fraction organic carbon using Equation 5.1. The sandy loam soil type is higher in weight percent organic matter in comparison with the other soil types. The default distribution type is Johnson SB; the minimum value is 0.0 and the maximum value is 11.0. A summary of this default distribution is presented in Table 3.9.

Table 3.9 Probability distribution of fraction organic carbon in the saturated zone

Cumulative Probability (%)	Fraction Organic Carbon in the Saturated Zone (unitless)
0.0	1.61E-05
1.0	1.31E-04
5.0	2.30E-04
10.0	4.31E-04
25.0	8.00E-04
50.0	9.27E-04
75.0	1.10E-03
90.0	1.35E-03
95.0	1.88E-03
100.0	1.24E-02

Data Sources

The default distribution described above for the fraction organic carbon in the saturated zone is based on data presented in Carsel, Parrish, Jones, Hansen, and Lamb, 1988.

Use In EPACMTP

The fraction organic carbon in the saturated zone is one of the most important subsurface parameters controlling the mobility of metals, since it is used in determining the extent to which a constituent's transport through the ground-water pathway is retarded due to adsorption. .

3.3.3.2.7 Ground-water Type (IGWT)***Definition***

Ground-water chemistry exerts an important influence on metal partition coefficients. The major ions present in ground water may compete with trace metals for sorption sites. Also, inorganic ligands may complex with some metals, thereby reducing their tendency to sorb. For the purposes of this modeling, partition coefficients were estimated separately for two ground-water compositional types, one with composition representative of a carbonate-terrain system and one representative of a non-carbonate system. The two ground-water compositional types are correlated with the hydrogeologic environment index in EPACMTP (see Section 5.3.4.2). In EPACMTP, this parameter may take on one of thirteen values, but issues of practicality limit the number of ground-water types for which separate partition coefficients can be estimated to just two. The broadest division of ground waters that may be made for the thirteen hydrogeologic environments in EPACMTP is carbonate and non-carbonate types of ground waters. Thus, these are the two broad types for which coefficients were estimated.

Parameter Value or Distribution of Values

By default, the ground-water type is directly correlated to the hydrogeologic environment setting in EPACMTP. In the default databases of WMU sites that have been compiled into auxiliary input files (called the site data files), each WMU site has been classified by the predominant hydrogeologic environment at the site. In EPACMTP, there are thirteen possible hydrogeologic environments. For the “solution limestone” hydrogeologic environment setting (IGWR = 12), the ground-water type is set to carbonate. The ground-water type for the other twelve possible hydrogeologic settings in EPACMTP are represented by the non-carbonate ground-water type.

Data Sources

The ground-water type is simply an arbitrary number assigned to provide a simple means of specifying which set of isotherms should be used (there is one set for carbonate ground water and another set for non-carbonate ground water). For both ground-water types, a representative, charge-balanced ground-water chemistry specified in terms of major ion concentrations and natural pH was selected from the literature. The carbonate system was represented by a well sample reported for a limestone aquifer (Freeze and Cherry, 1979). This ground water had a natural pH of 7.5 and was saturated with respect to calcite. The non-carbonate system was represented by a sample reported from an unconsolidated sand and gravel aquifer with a natural pH of 7.4 (White, Hem, and Waring, 1963). An unconsolidated sand and gravel aquifer was selected to represent the non-carbonate compositional type because it is the most frequently occurring of the twelve (non-carbonate) hydrogeologic environments in EPACMTP. More details about the MINTEQA2 modeling methodology and the compositions of both the carbonate and non-carbonate representative ground-water samples are presented in Appendix B.1.

Use In EPACMTP

The ground-water type is one of the most important subsurface parameters controlling the mobility of metals, since the major ions present in ground water may compete with trace metals for sorption sites. This may result in less availability of sorption sites for contaminants as they enter the ground water.

4.0 INFILTRATION AND RECHARGE PARAMETERS

This section discusses the individual parameters related to infiltration and recharge that are required to perform a modeling analysis using EPACMTP. Although most applications of EPACMTP are conducted on a national or regional basis for regulatory development purposes, EPACMTP can also be used in a location or a waste-specific mode. In either case, each of the input parameters related to the climatic characteristics of the site(s) being modeled can be specified as a constant value or as a statistical or empirical distribution of values. As a practical matter, however, many of these inputs are commonly specified as distributions of values as part of the regional site-based modeling methodology.

In EPACMTP, the infiltration and recharge-related input parameters include the climate center location, infiltration and recharge rates, and the soil and aquifer temperature. The climate center location is specified as an index that represents the climate center nearest to the waste site being modeled. The climate center index allows the model to access a default set of infiltration and recharge rates that are specific to a WMU type, soil type, and geographic location.

The infiltration rate is defined as the rate at which leachate flows from the bottom of the WMU (including any liner) into the unsaturated zone beneath the WMU. Recharge is the regional rate of aquifer recharge outside of the WMU. Infiltration rate is among the most sensitive site-specific parameters in an EPACMTP evaluation, whereas the model is usually much less sensitive to recharge. For landfills (LFs), waste piles (WPs), and land application units (LAUs), the infiltration rate is determined primarily by the local climatic conditions, especially annual precipitation and WMU liner characteristics. For SIs, the infiltration rate is a function of the surface impoundment ponding depth, liner characteristics, and the presence of a 'sludge' layer at the bottom of the impoundment. The regional recharge rate is a function of the annual precipitation rate, and varies with geographical location and soil type.

These infiltration and recharge-related parameters are individually described in the following sections.

4.1 INFILTRATION AND RECHARGE PARAMETERS

The input parameters that are used in EPACMTP to describe the climatic characteristics of the WMU site to be modeled are listed in Table 4.1 on the following page.

Table 4.1 Climate Parameters

Parameter	Symbol	Units	Section	Equation in EPACMTP TBD
Climate Center Index	<i>ICLR</i>	–	4.2	--
Landfill Infiltration Rate	<i>I</i>	m/yr	4.3.1	3.4
Waste Pile Infiltration Rate	<i>I</i>	m/yr	4.3.2	3.4
Land Application Unit Infiltration Rate	<i>I</i>	m/yr	4.3.3	3.4
Surface Impoundment Infiltration Rate	<i>I</i>	m/yr	4.3.4	2.24
Recharge Rate	<i>I_R</i>	m/yr	4.4	4.10

4.2 CLIMATE CENTER INDEX (ICLR)

Definition

The climate center index is simply a sequential number assigned to each of 102 climate centers in the default database included with EPACMTP in order to provide a simple means of specifying which infiltration and recharge rates should be used to model the given WMU site.

Parameter Value or Distribution of Values

The climate centers for which default infiltration rates (for LFs, WPs, and LAUs) and recharge rates (for LFs, WPs, SIs, and LAUs) are available are listed in Table 4.2. The geographic locations are depicted in Figure 4.1. For each of the locations listed in Table 4.2, the U.S. EPA used the Hydrologic Evaluation of Landfill Performance (HELP) model (Schroeder, Dozier, Zappi, McEnroe, Sjostrom, and Peton, 1994) to compute recharge rates for all units, as well as infiltration rates for LAUs and for LFs and WPs with no-liner and single-liner designs. Appendix A provides additional information about how EPA used the HELP model, in conjunction with data from climate stations across the United States, to develop these nationwide recharge and infiltration rate distributions, as well as a detailed discussion of how infiltration rates were developed for different liner designs for each type of WMU.

In developing this default distribution of infiltration rates, we started with an existing database of no-liner infiltration rates for LFs, WPs and LAUs. Also existing were recharge rates for 97 climate stations in the lower 48 contiguous United States (ABB, 1995), that are representative of 25 specific climatic regions (developed with HELP version 3.03). We then added five climate stations (located in Alaska, Hawaii, and Puerto Rico) to ensure coverage throughout all of the United States. Rather than calculating infiltration rates for each of the 102 individual climate stations,

infiltration rates were calculated for the 25 climate regions, and then assigned the same value to each climate station in one group. In order to reduce the number of required HELP simulations, one station from each climate region was simulated, and the resulting value assigned to each climate station within the region. To be protective, EPA chose the climate center with the highest average precipitation in each climate region (which would tend to maximize constituent transport) to represent the region. Individual infiltration rates were calculated for each of the five climate centers not assigned to a climate region (centers from Alaska, Hawaii, and Puerto Rico).

Table 4.2 Climate Centers Used in the HELP Modeling to Develop Infiltration and Recharge Rates

Index	City	State	Index	City	State	Index	City	State
1	Fresno	CA	29	Dodge City	KS	57	Tampa	FL
2	Boise	ID	30	Midland	TX	58	San Antonio	TX
3	Denver	CO	31	St. Cloud	MN	59	Hartford	CT
4	Grand Junction	CO	32	E. Lansing	MI	60	Syracuse	NY
5	Pocatello	ID	33	North Omaha	NE	61	Worcester	MA
6	Glasgow	MT	34	Tulsa	OK	62	Augusta	ME
7	Bismarck	ND	35	Brownsville	TX	63	Providence	RI
8	Pullman	WA	36	Dallas	TX	64	Portland	ME
9	Yakima	WA	37	Oklahoma City	OK	65	Nashua	NH
10	Cheyenne	WY	38	Concord	NH	66	Ithaca	NY
11	Lander	WY	39	Pittsburgh	PA	67	Boston	MA
12	Los Angeles	CA	40	Portland	OR	68	Schenectady	NY
13	Sacramento	CA	41	Caribou	ME	69	Lynchburg	VA
14	San Diego	CA	42	Chicago	IL	70	New York City	NY
15	Santa Maria	CA	43	Burlington	VT	71	Philadelphia	PA
16	Ely	NV	44	Bangor	ME	72	Seabrook	NJ
17	Rapid City	SD	45	Rutland	VT	73	Indianapolis	IN
18	Cedar City	UT	46	Seattle	WA	74	Cincinnati	OH
19	Albuquerque	NM	47	Montpelier	VT	75	Bridgeport	CT
20	Las Vegas	NV	48	Sault St. Marie	MI	76	Orlando	FL
21	Phoenix	AZ	49	Put-in-Bay	OH	77	Greensboro	NC
22	Tucson	AZ	50	Madison	WI	78	Jacksonville	FL
23	El Paso	TX	51	Columbus	OH	79	Watkinsville	GA
24	Medford	OR	52	Cleveland	OH	80	Norfolk	VA
25	Great Falls	MT	53	Des Moines	IA	81	Shreveport	LA
26	Salt Lake City	UT	54	E. St. Louis	IL	82	Astoria	OR
27	Grand Island	NE	55	Columbia	MO	83	New Haven	CT
28	Flagstaff	AZ	56	Topeka	KS	84	Plainfield	MA
85	Knoxville	TN	91	Tallahassee	FL	97	Miami	FL
86	Central Park	NY	92	New Orleans	LA	98	Annette	AK
87	Lexington	KY	93	Charleston	SC	99	Bethel	AK

Index	City	State	Index	City	State	Index	City	State
88	Edison	NJ	94	W. Palm Beach	FL	100	Fairbanks	AK
89	Nashville	TN	95	Atlanta	GA	101	Honolulu	HI
90	Little Rock	AK	96	Lake Charles	LA	102	San Juan	PR

Data Sources

The list of available climate centers was determined by the availability of meteorological data required for the HELP model and geographic coverage of the United States.

Use In EPACMTP

EPACMTP includes a database of infiltration rates and regional recharge rates for 102 climate centers located throughout the United States. The climate center index is a sequential number assigned to each climate center in the default database included with EPACMTP in order to provide a simple means of specifying which infiltration and recharge rates should be used to model the given WMU site (See Appendix A for a discussion on the determination of infiltration and recharge rates).

This parameter is used as a part of the regional site-based modeling methodology, in which a number of parameters related to the characteristics of the waste site are drawn from a correlated set of data. These default databases of site-related parameters (one for each WMU type) are commonly referred to as the site data files. To perform a Monte Carlo analysis using the regional site-based modeling methodology, the climate center index is provided in the site data files as the default setting, which will ensure that the appropriate climatic data is used for each WMU site in the database. However, if a location-adjusted or quasi-site-specific analysis is being performed, this input can either be omitted from the input file (if site-specific infiltration and recharge rates are available) or assigned a climate center index that is most appropriate to make use of the default location- and soil-specific infiltration and recharge rates which are included in the site data file. Usually this is the nearest climate center. However, this is not always the case. Especially in coastal and mountain regions, the nearest climate center does not always represent conditions that most closely approximate conditions at a specific site.



4.3 **INFILTRATION RATES**

The EPACMTP model requires input of the net rate of vertical downward percolation of water and leachate through the unsaturated zone to the water table. Infiltration refers to the water that percolates through a WMU to the underlying soil, whereas recharge is water percolating through the soil to the aquifer outside the footprint of the WMU. The model allows the infiltration rate to be different from the ambient regional recharge rate. These rates can differ for a variety of reasons, including the engineering design of the WMU, topography, land use, and vegetation. Note that both infiltration and recharge are specified as areal rates, with the units of cubic meters of fluid (water or leachate) per square meter per year ($\text{m}^3/\text{m}^2/\text{yr}$). Thus, the units for infiltration and recharge simplify to meters per year (m/yr).

Infiltration and recharge rates for use in EPACMTP modeling applications have been estimated for selected soil types at cities around the country through the use of the HELP water-balance model (Version 3.03) (Schroeder et al., 1994), as summarized below. Further details about the HELP modeling inputs, assumptions for each type of WMU, and the resulting databases of infiltration and recharge rates are given in Appendix A.

Using the Soil Conservation Service's (SCS) county-by-county soil mapping database, the soil classifications in the U.S. were grouped according to the U.S. Department of Agriculture's definitions of coarse, medium, and fine textures. These three categories are represented in EPACMTP by soils equivalent in properties to sandy loam (SNL), silt loam (SLT), and silty clay loam (SCL). An analysis of the SCS database indicates that coarse grained soils, medium grained soils, and fine grained soils represent 15.4 percent, 56.6 percent, and 28.0 percent, respectively, of the soils that have been mapped by the SCS.

The National Oceanic and Atmospheric Administration (NOAA) has data on precipitation and evaporation rates in the United States. This nationwide database was used to categorize the meteorological conditions in the U. S. into 18 climatic regions; 102 cities covering all 18 of the climatic regions were selected as climatic centers for the HELP model (Figure 4.1). For each selected city, climatic data for five years were accessed and used to develop leaching rates for different types of waste management scenarios as a function of site location and soil type. The resulting HELP-model-generated infiltration and recharge rates are incorporated into EPACMTP.

EPACMTP provides default values for infiltration rate as a function of WMU type, liner design, and site location. These values were calculated for unlined and single-lined landfills, waste piles, and land application units for each of the 102 climatic centers with the HELP model, using the procedure described in Appendix A. For composite-lined landfills and waste piles, these values are chosen from an empirical distribution of values based on the results of a literature review (TetraTech, 2001). In the case of surface impoundments, EPACMTP directly calculates the infiltration rate as a function of WMU characteristics, including liner type.

Because the infiltration rate from a WMU is difficult to measure directly, a model such as HELP is used to estimate the WMU infiltration rates for use in EPACMTP.

The data sources for infiltration rates for each type of WMU and the resulting infiltration rates are summarized in the following sections.

4.3.1 Landfill Infiltration Rate (I)

Definition

The landfill infiltration rate (m/yr) is defined as the rate at which water/leachate percolates through the landfill to the underlying soil. The landfill infiltration rate may be different from the ambient regional recharge rate due to the engineering design of the landfill (e.g., landfill cover soil that has a lower conductivity than the regional soils), topography, land use, and vegetation.

For the no-liner case, a two-foot (0.61m) soil cover was assumed to represent Subtitle D landfills that do not contain a liner and leak detection system, and therefore would not be required by the regulations to have a cap of less permeability than the liner system. Two feet was selected as the thickness of the cover as the minimum requirement of Subtitle D. Three default soil types were selected: sandy loam, silt loam, and silty clay loam, corresponding to the coarse, medium, and fine grained soil types as described in Section 4.3. These three soil types are assumed to support vegetation in the United States and are the three soil types used in the leachate flux analysis performed in support of the TC Rule modeling analysis (U.S. EPA, 1990).

For the single-clay liner case, a 3-ft. (0.914m) clay cover with a hydraulic conductivity of 1×10^{-7} cm/sec, a 1-ft. (0.305m) layer of loam overlying the cover (to support vegetation and drainage), a 10-ft. (3.05m) waste layer, a 1-ft. (0.305m) percolation layer, and a 3-ft. (0.914m) clay liner with a hydraulic conductivity of 1×10^{-7} cm/sec were specified in the HELP model input file. Additionally, the modeling assumed that there is no leachate collection system and that the infiltration rate is constant (that is, no increase in hydraulic conductivity of liner) over the modeling period.

A composite liner was defined as a 60 mil HDPE layer with either an underlying geosynthetic clay liner with maximum hydraulic conductivity of 5×10^{-9} cm/sec, or a 3-ft. (0.914m) compacted clay liner with maximum hydraulic conductivity of 1×10^{-7} cm/sec. As in the single-clay liner case, this scenario assumes a constant infiltration rate (i.e., no increase in hydraulic conductivity of liner) over the modeling period.

Parameter Value or Distribution of Values

When the EPACMTP model is run for an unlined or single-lined landfill using the regional, site-based methodology, the model selects a site at random from those in the site data file for each Monte Carlo realization. Since the landfill cover and soil

type for the landfills in the *1986 Subtitle D Survey* were unknown, a random combination of landfill cover soil type and regional soil type are then generated from a national joint probability distribution (assuming that the relative frequency of different soil and cover types is nationally uniform) (U.S.EPA, 1990). The climate center index associated with the chosen site and the randomly generated soil types are then used by the model to determine the recharge and infiltration values of the site from the HELP database also included in the site data file. In the case of unlined landfills, if the cover type and soil type underneath the unit are the same, the infiltration rate will be identical to the regional recharge rate for that soil type.

The cumulative frequency distributions of LF infiltration for the three default liner scenarios are presented in Table 4.3, and are based on the estimates described in the following sections; the LF infiltration rates for each climate center are presented in Appendix A.

Table 4.3 Cumulative Frequency Distribution of Landfill Infiltration

%	No Liner Infiltration Rate (m/yr)	Clay Liner Infiltration Rate (m/yr)	Composite Liner Infiltration Rate (m/yr)
0	1.00E-05	1.00E-05	0.00E+00
10	1.35E-02	9.44E-03	0.00E+00
25	6.58E-02	2.53E-02	0.00E+00
50	1.09E-01	4.32E-02	0.00E+00
75	2.74E-01	4.45E-02	7.30E-05
80	3.12E-01	4.77E-02	7.30E-05
85	3.53E-01	4.77E-02	1.12E-04
90	4.11E-01	4.86E-02	1.69E-04
95	4.56E-01	4.86E-02	2.83E-04
100	1.08E+00	5.26E-02	4.01E-04

Data Sources

The HELP model (Schroeder, et al., 1994) was used to estimate the rate at which leachate emanates from the base of the landfill for the no-liner and single-clay liner scenarios, using the procedure described in Appendix A.

For the composite liner case, the EPACMTP model randomly selects an infiltration rate from a default database of values which were compiled from a literature review of leak detection system flow rates (TetraTech, 2001).

When the EPACMTP model is run for a composite-lined landfill using the regional, site-based methodology, the model selects an infiltration rate at random from those in the default distribution for each Monte Carlo realization.

In a location-specific modeling analysis, the site-specific infiltration rate can

be directly specified in the input file – either as a constant value or as a statistical or empirical distribution of values.

Use In EPACMTP

The landfill infiltration rate is used by the model to determine the leaching duration and leachate concentration when the landfill depleting source option is used. Infiltration rate is also used by the model to determine the leachate flux to the subsurface and as an input to the subsurface flow and transport modules.

4.3.2 Waste Pile Infiltration Rate (I)

Definition

The waste pile infiltration rate is defined as the rate at which water/leachate percolates through the waste pile to the underlying soil. The waste pile infiltration rate may be different from the ambient regional recharge rate due to the engineering design of the waste pile (e.g., uncovered waste has a different conductivity than the regional soils), topography, land use, and vegetation.

For the purposes of estimating leaching rates using the HELP model, waste piles were considered to be similar to non-covered landfills. Thus, the infiltration rates for unlined and single-lined waste piles were generated using the same general procedures as for landfills, but with the following modifications. Because of the limited requirements for leachate collection systems in most states, after closure, waste piles will approximate the landfill configuration selected for modeling, i.e., waste covered by two feet of soil. Modeling of closed waste piles was, therefore, not necessary as their leaching characteristics are similar to closed landfills. Active waste piles, however, differ from landfills in that the waste generally remains uncovered. So the HELP model was used to model the leachate flux for waste piles through active, uncovered piles without leachate collection systems.

For the unlined scenario, the waste piles were modeled as a one-layer landfill, with the uncovered waste material comprising the layer. The waste material was assumed to be a moderate permeability waste – coal bottom ash with a permeability of 4.1×10^{-4} cm/sec.

For the single-lined scenario, an additional parameter – waste type permeability – is used. Since waste piles are not typically covered, the permeability of the waste itself can be a factor in determining the rate of leachate released due to water percolating through the WMU. For waste piles, the HELP modeling was conducted using three categories of waste permeability: high permeability (0.041 cm/sec); moderate permeability (0.0041 cm/sec); and low permeability (0.00005 cm/sec). The waste permeability is generally correlated with the grain size of the waste material, ranging from coarse- to fine-grained materials. Additionally, the modeling assumed that there is no leachate collection system and that the infiltration rate is constant (that is, no increase in hydraulic conductivity of liner) over the modeling period.

For the composite-lined scenario, the EPACMTP model randomly selects an infiltration rate from a default database of values which were compiled from a literature review of leak detection system flow rates (TetraTech, 2001). For the purposes of this literature review, a composite liner was defined as a 60 mil HDPE layer with either an underlying geosynthetic clay liner with maximum hydraulic conductivity of 5×10^{-9} cm/sec, or a 3-ft.(0.914m) compacted clay liner with maximum hydraulic conductivity of 1×10^{-7} cm/sec. As in the single-clay liner case, this scenario assumes a constant infiltration rate (i.e., no increase in hydraulic conductivity of liner) over the modeling period.

Parameter Value or Distribution of Values

The cumulative frequency distributions of WP infiltration for the three default liner scenarios are presented in Table 4.4, based on the estimates described in the following section; the WP infiltration rates for each climate center are presented in Appendix A.

Table 4.4 Cumulative Frequency Distribution of Waste Pile Infiltration

%	No Liner Infiltration Rate (m/yr)	Clay Liner Infiltration Rate (m/yr)	Composite Liner Infiltration Rate (m/yr)
0	3.00E-04	1.00E-05	0.00E+00
10	6.02E-02	2.64E-02	0.00E+00
25	1.28E-01	9.50E-02	0.00E+00
50	2.55E-01	1.27E-01	0.00E+00
75	3.91E-01	1.33E-01	7.30E-05
80	4.49E-01	1.33E-01	7.30E-05
85	4.76E-01	1.34E-01	1.16E-04
90	5.38E-01	1.35E-01	1.67E-04
95	6.14E-01	1.35E-01	2.80E-04
100	1.82E+00	1.36E-01	4.01E-04

Data Sources

The HELP model (Schroeder et. al., 1994) was used to estimate the rate at which leachate emanates from the base of the waste pile for the no-liner and single-clay liner scenarios. This modeling methodology is summarized here and is more fully described in Appendix A.

Use In EPACMTP

When the EPACMTP model is run for an unlined or single-lined waste pile using the regional, site-based methodology, the model selects a site at random from those in the site data file for each Monte Carlo realization. The climate center index associated with the chosen site and the randomly generated soil types are then used by the model to determine the recharge and infiltration values of the site from the HELP databases also included in the site data file.

When the EPACMTP model is run for a composite-lined waste pile using the regional, site-based methodology, the model selects an infiltration rate at random from those in the default distribution for each Monte Carlo realization.

In a location-specific modeling analysis, the site-specific infiltration rate can be directly specified in the input file – either as a constant value or as a statistical or empirical distribution of values.

Once the waste pile infiltration rate is generated, it is used by the model to determine the leachate flux to the subsurface and as an input to the subsurface flow and transport modules.

4.3.3 Land Application Unit Infiltration Rate (I)***Definition***

The land application unit infiltration rate is defined as the rate at which water/leachate percolates through the land application unit to the underlying soil. Although the actual infiltration rate at a land application site may be slightly different from the ambient regional recharge rate due to the additional water in the land applied sludge, topography, land use, and vegetation, the default Monte Carlo analysis in EPACMTP assumes that these rates are identical.

Based upon sensitivity analyses using a range of waste application rates, EPA established that the addition of amounts of water through application of sludge-type wastes does not significantly impact the soil water balance, and therefore has little to no effect on the calculated net infiltration. Only for sites located in arid regions of the United States with very little natural precipitation did high application rates have an appreciable effect. For more representative waste application rates, the effect disappeared because introducing additional moisture in the simulated water balance resulted in a commensurate increase in runoff and removal by evapotranspiration.

Based on these results, the land application unit infiltration rates at the 102 climate centers were taken to be the same as the ambient regional recharge rate for that climatic center and soil type. In addition, the recharge rate for a given climate center and soil type is taken to be the same as the corresponding landfill infiltration rate.

Parameter Value or Distribution of Values

When the EPACMTP model is run for a land application unit using the regional, site-based methodology, the model selects a site at random from those in the site data file for each Monte Carlo realization. The climate center index associated with the chosen site and the randomly generated soil types are then used by the model to determine the recharge and infiltration values of the site from the HELP databases also included in the site data file.

The cumulative frequency distribution of LAU infiltration for the no-liner scenario is presented in Table 4.5, based on the estimates described in the following sections; the LAU infiltration rates for each climate center are presented in Appendix A.

Table 4.5 Cumulative Frequency Distribution of Land Application Unit Infiltration

%	No Liner Infiltration Rate (m/yr)
0	1.00E-05
10	1.30E-02
25	7.04E-02
50	1.10E-01
75	2.01E-01
80	2.57E-01
85	2.89E-01
90	3.26E-01
95	3.65E-01
100	7.45E-01

Data Sources

In a location-specific modeling analysis, the site-specific infiltration rate can be directly specified in the input file – either as a constant value or as a statistical or empirical distribution of values.

The HELP model was used to estimate the rate at which leachate emanates from the base of the land application unit for the no-liner scenario. This modeling methodology is summarized here and is more fully described in Appendix A.

Use In EPACMTP

Once the land application unit infiltration rate is generated, it is used by the model to determine the leachate flux to the subsurface and as an input to the subsurface flow and transport modules.

4.3.4 Surface Impoundment Infiltration Rate (I)

Definition

The surface impoundment infiltration rate is defined as the rate at which water/leachate percolates through the surface impoundment to the underlying soil. The surface impoundment infiltration rate is generally larger than the ambient regional recharge rate due to the hydraulic head created by the wastewater in the impoundment.

For the surface impoundment scenario, the leachate flux rate is computed as a derived parameter, as part of the unsaturated zone flow module in EPACMTP. The algorithm is described in the *EPACMTP Technical Background Document* (US EPA, 2003a). In a typical Monte Carlo modeling analysis of a surface impoundment, the infiltration rate is derived by the EPACMTP model. Technically, the SI infiltration rate is not really an input parameter; rather, the model calculates infiltration rates “on the fly” during the simulation. In the event that the SI is reported to have its base below the water table, EPACMTP calculates the infiltration using Darcy’s law based on the hydraulic gradient across and the hydraulic conductivity of the consolidated sediment and any liner material at the bottom of the impoundment unit. Based on unit-specific data from EPA’s Surface Impoundment Study (US EPA 2001a), EPA assumed a fixed sediment layer thickness of 20 cm at the base of the impoundment. In addition, the EPACMTP model assumes that the depth of clogging underneath the impoundment was 0.5 m in all cases, and that saturated hydraulic conductivity of the clogged layer is 10% of that of the native soil underlying the impoundment.

For unlined SIs, the primary parameters that control the infiltration rate are the ponding depth in the impoundment, the thickness and permeability of any accumulated sediment layer at the base of the impoundment, and the presence of a ‘clogged’ (i.e., reduced permeability) layer of native soil under the impoundment caused by the migration of solids from the impoundment.

For single-lined SIs, infiltration rates are typically calculated inside of EPACMTP in the same manner as described for unlined units, with the exception that a compacted clay liner (with a given thickness and hydraulic conductivity) is added at the bottom of the WMU and the effect of clogged native material is not included due to the filtering effects of the liner. For more information on the EPACMTP inputs used to describe the SI liner thickness and conductivity, see Sections 2.4.4. and 2.4.5.

For the composite-lined SI, the EPACMTP model determines its infiltration rate using a default distribution of leak densities expressed as number of leaks per hectare (see Section 2.4.7).

Parameter Value or Distribution of Values

When the EPACMTP model is run for any of the three default liners for the surface impoundment scenario using the regional, site-based methodology, the

model selects a site at random from those in the site data file for each Monte Carlo realization. Using the characteristics of the chosen site and the methods described above, the model automatically calculates the infiltration rate. The climate center index associated with the chosen site and the randomly generated soil types are then used to determine the recharge rate for the site from the HELP database also included in the site data file.

The cumulative frequency distributions of SI infiltration for the three default liner scenarios (produced by running a standard regional site-based modeling analysis) are presented in Table 4.6; the SI infiltration rates for each climate center are presented in Appendix A.

Table 4.6 Cumulative Frequency Distribution of Surface Impoundment Infiltration

%	No Liner Infiltration Rate (m/yr)	Clay Liner Infiltration Rate (m/yr)	Composite Liner Infiltration Rate (m/yr)
0	3.78E-15	3.78E-15	0.00E+00
10	2.71E-01	4.22E-02	0.00E+00
25	5.21E-01	6.29E-02	0.00E+00
50	1.14E+00	1.08E-01	4.88E-05
75	2.27E+00	1.63E-01	2.02E-04
80	2.58E+00	1.76E-01	2.67E-04
85	2.94E+00	1.94E-01	3.55E-04
90	3.51E+00	2.17E-01	4.98E-04
95	4.51E+00	2.69E-01	7.51E-04
100	2.23E+01	7.98E-01	3.69E-03

Data Sources

In a location-specific modeling analysis, the site-specific infiltration rate can be directly specified in the input file – either as a constant value or as a statistical or empirical distribution of values.

To create the surface impoundment site data file for use with EPACMTP, EPA used unit-specific data for SIs from EPA's *Surface Impoundment Study* (U.S. EPA, 2001a). The resulting sediment layer permeability has a relatively narrow range of variation between 1.26×10^{-7} and 1.77×10^{-7} cm/s. This database of surface impoundment sites is tabulated in Appendix D.

Default data on leak density were compiled from 26 leak density values reported in TetraTech (2001). Further details of the methodology and data used to derive SI infiltration for the composite liner scenario are presented in Section 4.2.2.4 of the *IWEM Technical Background Document* (U.S. EPA, 2003c).

Use In EPACMTP

The surface impoundment infiltration rate is used by the model to determine the leachate flux to the subsurface and as an input to the subsurface flow and transport modules.

4.4 RECHARGE RATE (I_R)***Definition***

The recharge rate is the rate at which water percolates through the soil to the water table outside the footprint of the WMU. The recharge rate is determined by regional climatic conditions, such as precipitation, evapotranspiration, surface run-off, and regional soil type. The ambient regional rate may be different from the infiltration rate through the WMU due to the engineering design of the unit (e.g., landfill cover soil of a different type, hydraulic head of the impoundment, or low waste conductivity), topography, land use, and/or vegetation. The recharge rate is determined by the regional climatic and soil conditions, such as precipitation, evapotranspiration, surface run-off, and regional soil type. Note that both infiltration and recharge are specified as areal rates, with the units of cubic meters of fluid (water or leachate) per square meter per year ($\text{m}^3/\text{m}^2/\text{yr}$). Thus, the units for infiltration and recharge simplify to meters per year (m/yr).

Parameter Value or Distribution of Values

EPA created the database of recharge rates for the three primary soil types across the United States (SNL, SLT, and SCL) and ambient climate conditions at 102 climate stations through the use of the HELP water-balance model as presented in Appendix A. The ambient regional recharge rate for a given climate center and soil type (for all four WMU types) was assumed to be the same as the corresponding unlined LF infiltration rate. The cumulative frequency distribution of recharge (produced by running a standard regional site-based modeling analysis for a landfill) are presented in Table 4.7; the recharge rate for each climate center is presented in Appendix A.

Table 4.7 Cumulative Frequency Distribution of Regional Recharge Rate

%	Recharge Rate (m/yr)
0	1.00E-05
10	1.35E-02
25	6.86E-02
50	1.22E-01
75	3.08E-01
80	3.42E-01
85	3.90E-01
90	4.38E-01
95	4.67E-01
100	1.15E+00

Data Sources

The HELP model was used to estimate the ambient regional recharge rate, using the procedure described in Appendix A. Note that the recharge rate for a given climate center and soil type (for all 4 types of WMUs) is assumed to be the same as the corresponding unlined landfill infiltration rate (see Section 4.3.1.1).

Use In EPACMTP

When the EPACMTP model is run using the regional, site-based methodology, the model selects a site at random from those in the site data file for each Monte Carlo realization. The climate center index associated with the chosen site and the randomly generated soil type are then used by the model to determine the recharge value of the site from the HELP database also included in the site data file.

In a location-specific modeling analysis, the site-specific regional recharge rate can be directly specified in the input file – either as a constant value or as a statistical or empirical distribution of values.

Once the recharge rate is generated, it is used by the model as an input to the subsurface flow and transport modules.

5.0 HYDROGEOLOGICAL PARAMETERS

EPACMTP treats the subsurface aquifer system as a composite domain, consisting of an unsaturated (vadose) zone and an underlying saturated zone (an unconfined aquifer). The boundary between the two zones is the water table. The unsaturated zone and saturated zone modules are computationally linked through continuity of flow and constituent concentration across the water table directly underneath the waste management unit (WMU). The model accounts for the following processes affecting constituent fate and transport as the constituent migrates from the bottom of a WMU through the unsaturated and saturated zones: advection, hydrodynamic dispersion and molecular diffusion, linear or nonlinear equilibrium sorption, first-order decay and zero-order production reactions (to account for transformation breakdown products), and dilution due to recharge in the saturated zone.

This section discusses the individual hydrogeological parameters characterizing the soil and aquifer that are required to perform a modeling analysis using EPACMTP. Although most applications of EPACMTP are conducted on a national or regional basis for regulatory development purposes, EPACMTP can also be used in a location-specific mode. In either case, each of the input parameters describing the soil and aquifer beneath the waste site being modeled can be specified as a constant value or as a statistical or empirical distribution of values. As a practical matter, however, many of these inputs are commonly specified using a distribution of values.

There are a number of data sources available to obtain parameter values for the unsaturated and saturated zone modeling in EPACMTP. For unsaturated zone modeling, we used a database of soil hydraulic properties for various soil types, assembled by Carsel and Parrish (1988), in combination with information from the Soil Conservation Service (SCS) on the nationwide prevalence of different soil types across the United States. Another primary data source was the Hydrogeologic Database for Ground-Water Modeling (HGDB), assembled by Rice University on behalf of the American Petroleum Institute (API) (Newell, Hopkins, and Bedient, 1990). This database provides probability distributions of a number of key ground-water modeling parameters for various types of subsurface environments.

The HGDB was developed from a survey of the hydrogeologic characteristics at actual hazardous waste sites in the United States and provides site specific data on ground water parameters (aquifer thickness, unsaturated zone thickness, hydraulic gradient and hydraulic conductivity) collected by independent investigators for approximately 400 hazardous waste sites throughout the U.S. These site-specific data were then regrouped into 13 hydrogeologic environments, based on the USGS classification of aquifer regions (Heath, 1984) (12 specific environments and one category called "other"). The result is a database of aquifer types, with each aquifer type consisting of an empirical distribution of values for each of the four aquifer parameters.

These hydrogeological parameters are individually described in the following sections.

5.1 HYDROGEOLOGICAL PARAMETERS

The hydrogeological input parameters include parameters to characterize both the flow regime and constituent transport in both the unsaturated zone and aquifer in the vicinity of the modeled WMU. These parameters are listed in Table 5.1.

5.2 UNSATURATED ZONE PARAMETERS

In the unsaturated zone, EPACMTP simulates one-dimensional, vertically downward flow and transport of constituents between the base of the WMU and the water table. The unsaturated zone-specific model inputs used by the model to simulate the fate of constituents as they are transported through the subsurface include the unsaturated zone thickness, hydraulic conductivity and other hydraulic properties of the soil, the bulk density of the soil, the dispersivity in the unsaturated zone, percent organic matter, and parameters describing the sorption and/or degradation of the modeled constituent. The primary output from the unsaturated zone module is the predicted contaminant concentration entering the saturated zone at the water table, either as a function of time (the breakthrough curve) or at steady-state.

These unsaturated zone parameters are individually described in the following sections.

5.2.1 Unsaturated Zone Thickness (D_u)

Definition

The unsaturated zone thickness is the vertical distance from the ground surface to the water table. The water table in this case is meant to represent the 'natural' water elevation, as it is or would be without the influence from the WMU. The presence of a WMU, particularly a surface impoundment, may cause a local rise in the water table called mounding. The EPACMTP model assumes that the unsaturated zone thickness value you have entered does not include mounding. The model will calculate the predicted impact of the WMU and liner design (if any) on the ground water as part of the modeling evaluation.

Note that in cases where the WMU is excavated, such that the base of the unit is below ground surface, the unsaturated zone thickness should be the long-term average regional depth to ground water, measured outside the footprint of the WMU. The input variable *Depth Below Grade* (see Sections 2.3.3, 2.4.6, and 2.5.3) is used to correct the unsaturated zone thickness beneath an excavated WMU.

Table 5.1 Hydrogeological Parameters

Module	Parameter	Symbo l	Units	Section	Equation in EPACMTP Tech. Bkgd. Doc
Unsaturated Zone	Unsaturated Zone Thickness	D_u	m	5.2.1	3.9
	Soil Type Index	ISTYPE	unitless	5.2.2	
	Soil Hydraulic Conductivity	K_s	cm/hr	5.2.3.1	3.4
	Alpha	α	1/cm	5.2.3.2	3.1
	Beta	β	unitless	5.2.3.3	3.1
	Residual Water Content	θ_r	unitless	5.2.3.4	3.1
	Saturated Water Content	θ_s	unitless	5.2.3.5	3.1
	Soil Bulk Density	ρ_{bu}	g/cm ³	5.2.3.6	3.16
	Percent Organic Matter	%OM	unitless	5.2.3.7	3.10
	Dispersivity	α_{LU}	m	5.2.4	3.9
	Leading Coefficient of Freundlich Isotherm	K_d	cm ³ /g	5.2.5.1	3.11
	Exponent of Freundlich Isotherm	η	unitless	5.2.5.2	3.18
	Chemical Degradation Rate	λ_{cu}	1/yr	5.2.6	3.13
	Biodegradation Rate	λ_{bu}	1/yr	5.2.7	3.12
	Soil Temperature	T	°C	5.2.8	4.4.3.3
	Soil pH	pH	standard units	5.2.9	4.4.3.4
Saturated Zone	Particle Diameter	d	cm	5.3.1	4.1
	Porosity	ϕ	unitless	5.3.2	4.2
	Bulk Density	ρ_b	g/cm ³	5.3.3	4.3
	Hydrogeologic Environment Index	IGWR	unitless	5.3.4.2	
	Saturated Zone Thickness	B	m	5.3.4.3	2.31
	Hydraulic Conductivity	K	m/yr	5.3.4.4	4.4
	Regional Hydraulic Gradient	r	unitless	5.3.4.5	4.6
	Seepage Velocity	V_x	m/yr	5.3.5	4.6
	Anisotropy Ratio	A_r	unitless	5.3.6	4.5
	Retardation Coefficient	R^s	unitless	5.3.7	4.18
	Longitudinal Dispersivity	α_L	m	5.3.8.1	4.19

Module	Parameter	Symbol	Units	Section	Equation in EPACMTP Tech. Bkgd. Doc
Saturated zone	Horizontal Transverse Dispersivity	α_T	m	5.3.8.2	4.28
	Vertical Dispersivity	α_V	m	5.3.8.3	4.29
	Aquifer Temperature	T	°C	5.3.9	4.4.3.3
	Ground-water pH	pH	standard units	5.3.10	Section 4.4.3.4
	Fractional Organic Carbon Content	f_{oc}^s	unitless	5.3.11	4.30
	Leading Coefficient of Freundlich Isotherm	K_d^s	cm ³ /g	5.3.12	4.18
	Exponent of Freundlich Isotherm	n^s	unitless	5.3.13	4.34
	Chemical Degradation Rate	λ_c^s	1/yr	5.3.14	Section 4.4.3.9
	Biodegradation Rate	λ_b^s	1/yr	5.3.15	Section 4.4.3.9

Parameter Value or Distribution of Values

Lacking a site-specific value or distribution of values to input, a default distribution of unsaturated zone thickness values may be used as part of the regional site-based modeling methodology. As described in Section 5.5 of the *EPACMTP Technical Background Document* (U.S. EPA, 2003a), the regional site-based modeling methodology is an attempt to ensure that the combination of parameter values randomly generated by the Monte Carlo module of EPACMTP represents a realistic set of site conditions. The cumulative frequency distribution of unsaturated zone thickness listed in Table 5.2 was generated by performing a default landfill modeling analysis using the regional site-based modeling methodology; the entire Hydrogeologic Database for Modeling (HGDB) from which these values were derived is presented in Appendix D.

Table 5.2 Cumulative Frequency Distribution of Unsaturated Zone Thickness

%	Unsaturated Zone Thickness (m)
0	3.05E-01
10	1.68E+00
25	3.96E+00
50	6.10E+00
75	1.52E+01
80	1.83E+01
85	2.93E+01
90	4.27E+01
95	5.08E+01
100	6.10E+02

Data Sources

EPA obtained data on the unsaturated zone thickness from the Hydrogeologic Database for Modeling (HGDB; Newell et al., 1990; U.S. EPA, 1997d). A database of soil hydraulic properties for various soil types, assembled by Carsel and Parrish (1988) was also used, in combination with information from the Soil Conservation Service (SCS) on the nationwide prevalence of different soil types across the United States. The Hydrogeologic Database for Modeling (HGDB) from which the values shown in Table 5.2 were derived is presented in its entirety in Appendix D.

In the regional site-based Monte Carlo analysis that is typically used for nationwide modeling applications, the resulting distribution of values for the thickness of the unsaturated zone is produced through Monte Carlo sampling of the HGDB, based on the hydrogeologic environment assigned to the waste site selected for each model realization. In a location-adjusted or quasi-site-specific modeling analysis, the site-specific unsaturated zone thickness can be directly specified as a constant value or an empirical or statistical distribution of values.

Use In EPACMTP

The EPACMTP model uses the unsaturated zone thickness to determine the travel distance of leachate constituents in the unsaturated zone.

5.2.2 Soil Type (ISTYPE)**Definition**

Soil type is a way to group or classify soils with similar properties. EPACMTP incorporates three soil types, sandy loam, silt loam, and silty clay loam, that represent the most prevalent soil types across the U.S.

The soil type is indicated by a numerical index which is simply a sequential number assigned to each soil type in the default database included with EPACMTP in order to provide a simple means of specifying which distributions should be used to generate the input values for the soil characteristics required to run the model.

Parameter Value or Distribution of Values

The soil types for which default data are available are listed in Table 5.3; the corresponding soil parameter distributions are summarized in Section 5.2.3. When performing a regional site-based modeling analysis of a landfill, waste pile, or land application unit, the soil type is randomly chosen based on the nationwide frequency of occurrence, based on Soil Conservation Service (SCS) soil mapping data. These percentages are shown below in Table 5.3. When performing a regional site-based modeling analysis of a WMU, the soil type for each unit is specified in the default site data file.

Table 5.3 Default EPACMTP Soil Types

Soil Type Index	Texture	Soil Name	Abbreviation	Frequency of Occurrence
1	medium	silt loam	SLT	56.6%
2	coarse	sandy loam	SNL	15.4%
3	fine	silty clay loam	SCL	28%

Data Sources

Parameter distributions for soil parameters were compiled by Carsel and Parrish (1988). Information on the relative frequency of each soil type was obtained from the U.S. Soil Conservation Service as part of the risk analysis in support of EPA's development of the Toxicity Characteristic Final Rule (U.S. EPA, 1990).

Use In EPACMTP

To perform a typical Monte Carlo analysis using the regional site-based modeling methodology, the soil type index should be left in its default setting, ensuring that the appropriate climatic data is used for each WMU site in the database. However, if a location-specific analysis is being performed, then this input can either be omitted from the input file (if site-specific values for the soil characteristics are available) or set to the appropriate constant value to make use of the default soil data which are included in the model.

5.2.3 Soil Hydraulic Characteristics

EPACMTP uses the so-called van Genuchten model to describe the soil hydraulic characteristics. The parameters used to describe the soil hydraulic characteristics include residual water content, saturated water content, and two van Genuchten empirical water soil moisture parameters (α and β).

Solution of the unsaturated zone flow requires knowledge of the soil characteristic curves, i.e., the relationship between water saturation and pressure head and between hydraulic conductivity and water saturation. The van Genuchten (1980) model is widely used for predicting soil-water content as a function of pressure head. Descriptive statistical values for the parameters used in this model have been determined by Carsel and Parrish (1988) for 12 soil classifications. The statistical distributions for the parameters presented in Carsel and Parrish (1988) (as well as the bulk density and percent organic matter from Carsel et al., 1988) for the three default soil types used in EPACMTP are presented in Table 5.4. The variables analyzed by Carsel and Parrish include saturated hydraulic conductivity (K_s), residual water content (θ_r), saturated water content (θ_s), and three empirical constants (α , β , and γ). Probability distributions for α , β , and γ for all 12 soil types from Carsel and Parrish (1988) are presented in Table 5.6.

5.2.3.1 Soil Hydraulic Conductivity (K_s)

Definition

The hydraulic conductivity of the soil is a measure of the soil's ability to transmit water under fully saturated conditions.

Parameter Value or Distribution of Values

If site-specific data are available, then the soil hydraulic conductivity can be specified as a constant value or an empirical or statistical distribution of values.

Table 5.4 Statistical parameters for soil properties for three soil types used in the EPACMTP model (Carsel and Parrish, 1988 and Carsel et al., 1988). All values are in arithmetic space

Distribution		Limits of Variation		Standard	
Variable	Type	Minimum	Maximum	Mean	Deviation
Soil Type - Silty Clay Loam					
K_s cm/hr	SB	0.	3.5	0.017	2.921
θ_r	NO	0.00	0.115	0.089	0.0094
α cm ⁻¹	SB	0.00	0.15	.009	.097
β	NO	1.0	1.5	1.236	0.061
% OM	SB	0.0	8.35	0.11	5.91
ρ_b	Constant	-	-	1.67	-
θ_s	Constant	-	-	0.43	-
Soil Type - Silt Loam					
K_s cm/hr	LN	0.	15.0	.343	.989
θ_r	SB	0.00	0.11	.068	0.071
α cm ⁻¹	LN	0.00	0.15	.019	0.012
β	SB	1.0	2.0	1.409	1.629
% OM	SB	0.0	8.51	0.105	5.88
ρ_b	Constant	-	-	1.65	-
θ_s	Constant	-	-	0.45	-
Soil Type - Sandy Loam					
K_s cm/hr	SB	0.	30.0	2.296	24.65
θ_r	SB	0.	0.11	0.065	0.074
α cm-1	SB	0.	0.25	0.070	0.171
β	LN	1.35	3.00	1.891	0.155
% OM	SB	0.0	11.0	0.074	7.86
ρ_b	Constant	-	-	1.60	-
θ_s	Constant	-	-	0.41	-

% OM = Percent Organic Matter

NO = Normal distribution

SB = Log ratio distribution, $Y = \ln [(x-A)/(B-x)]$, $A < x < B$

LN = Log normal distribution, $Y = \ln[x]$

where Y = normal distributed parameter

x = actual data

K_s = Saturated Hydraulic Conductivity

θ_r = Residual water content

α, β = van Genuchten parameters

ρ_b = Bulk density

θ_s = Saturated Water Content

Lacking site-specific data, a default distribution of soil hydraulic conductivity values may be used as part of the regional site-based modeling methodology (see Section 5.5 of the *EPACMTP Technical Background Document* (U.S. EPA, 2003a)). The EPACMTP model includes a database of soil characteristics for each of three default soil types; hydraulic conductivity is one of the soil characteristics included in these default databases. A statistical summary of the values used for each of the three default soil types, including hydraulic conductivity, is shown in Table 5.4, above. The cumulative frequency distribution of soil hydraulic conductivity values listed in Table 5.5 was generated by performing a default nationwide landfill modeling analysis using the regional site-based modeling methodology. For a given percentile (%) frequency and value pair in Table 5.5, the percentile denotes the relative frequency or likelihood of parameter values in the entire distribution being less than or equal to the corresponding parameter value in the right hand column.

Table 5.5 Cumulative Frequency Distribution of Soil Hydraulic Conductivity

%	Soil Hydraulic Conductivity (cm/hr)
0	4.30E-05
10	6.79E-03
25	2.33E-02
50	8.90E-02
75	3.99E-01
80	6.09E-01
85	9.97E-01
90	1.93E+00
95	4.41E+00
100	2.79E+01

Data Sources

The databases of soil characteristics for the three default soil types (which include soil hydraulic conductivity) were derived from soil hydraulic property data reported by Carsel and Parrish (1988).

Use In EPACMTP

The hydraulic conductivity of the soil is used as an input to the unsaturated zone flow module and is used to calculate the moisture content in the soil under a given rate of leachate infiltration from the WMU.

Table 5.6 Descriptive statistics for van Genuchten water retention model parameters, α , β , and γ (Carsel and Parrish, 1988)

	Parameter α , cm ⁻¹					Parameter β					Parameter γ			
Soil Type	X	SD	CV	N		X	SD	CV	N		X	SD	CV	N
Clay ^a	0.008	0.012	160.3	400		1.09	0.09	7.9	400		0.08	0.07	82.7	400
Clay Loam	0.019	0.015	77.9	363		1.31	0.09	7.2	364		0.24	0.06	23.5	364
Loam	0.036	0.021	57.1	735		1.56	0.11	7.3	735		0.36	0.05	13.5	735
Loamy Sand	0.124	0.043	35.2	315		2.28	0.27	12.0	315		0.56	0.04	7.7	315
Silty Clay	0.005	0.005	113.6	126		1.09	0.06	5.0	374		0.08	0.05	51.7	374
Silty Clay Loam	0.010	0.006	61.5	641		1.23	0.06	5.0	641		0.19	0.04	21.5	641
Silt	0.016	0.007	45.0	82		1.37	0.05	3.3	82		0.27	0.02	8.6	82
Silt Loam	0.020	0.012	64.7	1093		1.41	0.12	8.5	1093		0.29	0.06	19.9	1093
Sandy Clay	0.027	0.017	61.7	46		1.23	0.10	7.9	46		0.19	0.06	34.7	46
Sandy Clay Loam	0.059	0.038	64.6	214		1.48	0.13	8.7	214		0.32	0.06	53.0	214
Sandy Loam	0.075	0.037	49.4	1183		1.89	0.17	9.2	1183		0.47	0.05	10.1	1183
Sand	0.145	0.029	20.3	246		2.68	0.29	20.3	246		0.63	0.04	6.3	246

N = Sample size, X = Mean

SD = Standard Deviation

CV = Coefficient of Variation (percent)

^a = Agricultural Soil, Clay 60 percent

$\gamma = 1 - 1/\beta$

5.2.3.2 Alpha (α)

Definition

Alpha is a soil-specific shape parameter that is obtained from an empirical relationship between pressure head and volumetric water content; it is one of the parameters in the van Genuchten (1980) model used for modeling soil-water content as a function of pressure head, and is used to calculate the moisture content in the soil under a given rate of leachate infiltration from the WMU.

Parameter Value or Distribution of Values

If site-specific data are available, then the van Genuchten parameter alpha can be specified in the input file as a constant value or an empirical or statistical distribution of values.

Lacking site-specific data, a default distribution of soil hydraulic conductivity values may be used as part of the regional site-based modeling methodology (see Section 5.5 of the *EPACMTP Technical Background Document* (U.S. EPA, 2003a)). The EPACMTP model includes a database of soil characteristics for each of three default soil types; van Genuchten parameter alpha is one of the soil characteristics included in these default databases. A statistical summary of the values used for each of the three default soil types, including the van Genuchten parameter alpha, is shown in Table 5.4. The cumulative frequency distribution of soil hydraulic conductivity values listed in Table 5.7 was generated by performing a default nationwide landfill modeling analysis using the regional site-based modeling methodology. For a given percentile (%) frequency and value pair in Table 5.7, the percentile denotes the relative frequency or likelihood of parameter values in the entire distribution being less than or equal to the corresponding parameter value in the right hand column.

Table 5.7 Cumulative Frequency Distribution of Alpha

%	Alpha (1/cm)
0	1.29E-03
10	5.96E-03
25	9.35E-03
50	1.52E-02
75	2.71E-02
80	3.26E-02
85	4.22E-02
90	5.90E-02
95	8.92E-02
100	2.18E-01

Data Sources

The databases of soil characteristics for the three default soil types (which include the van Genuchten parameter (α)) were derived from soil hydraulic property data reported by Carsel and Parrish (1988).

Use In EPACMTP

The van Genuchten parameter alpha is an input to the unsaturated zone flow module and is used to calculate the moisture content in the soil under a given rate of leachate infiltration from the WMU.

5.2.3.3 Beta (β)**Definition**

Beta is a soil-specific shape parameter that is obtained from an empirical relationship between pressure head and volumetric water content; it is one of the parameters in the van Genuchten (1980) model used for modeling soil-water content as a function of pressure head.

Parameter Value or Distribution of Values

If site-specific data are available, then the van Genuchten parameter beta can be specified in the input file as a constant value or an empirical or statistical distribution of values.

Lacking site-specific data, a default distribution of soil hydraulic conductivity values may be used as part of the regional site-based modeling methodology (see Section 5.5 of the *EPACMTP Technical Background Document* (U.S. EPA, 2003a)). The EPACMTP model includes a database of soil characteristics for each of three default soil types; van Genuchten parameter beta is one of the soil characteristics included in these default databases. A statistical summary of the values used for each of the three default soil types, including the van Genuchten parameter beta, is shown in Table 5.4. The cumulative frequency distribution of soil hydraulic conductivity values listed in Table 5.8 was generated by performing a default nationwide landfill modeling analysis using the regional site-based modeling methodology. For a given percentile (%) frequency and value pair in Table 5.8, the percentile denotes the relative frequency or likelihood of parameter values in the entire distribution being less than or equal to the corresponding parameter value in the right hand column.

Table 5.8 Cumulative Frequency Distribution of Beta

%	Beta (unitless)
0	1.03E+00
10	1.20E+00
25	1.27E+00
50	1.37E+00
75	1.53E+00
80	1.58E+00
85	1.68E+00
90	1.82E+00
95	1.96E+00
100	2.50E+00

Data Sources

The databases of soil characteristics for the three default soil types (which include the van Genuchten parameter (β)) were derived from soil hydraulic property data reported by Carsel and Parrish (1988).

Use In EPACMTP

The van Genuchten parameter beta is an input to the unsaturated zone flow module and is used to calculate the moisture content in the soil under a given rate of leachate infiltration from the WMU.

5.2.3.4 Residual Water Content (θ_r)**Definition**

At atmospheric pressure, the saturated water content represents the maximum fraction of the total volume of soil that is occupied by the water contained in the soil. The soil will remain saturated as the pressure head is gradually decreased. Eventually, as the pressure head decreases to a threshold known as the bubbling pressure, the water will begin to drain from the soil. The moisture content will continue to decline as the pressure head is lowered until it reaches some irreducible residual water content. Should the pressure head be further reduced, the soil would not lose any additional moisture.

Parameter Value or Distribution of Values

If site-specific data are available, then the residual water content of the soil can be specified as a constant value or an empirical or statistical distribution of values.

Lacking site-specific data, a default distribution of soil hydraulic conductivity values may be used as part of the regional site-based modeling methodology (see

Section 5.5 of the *EPACMTP Technical Background Document* (U.S. EPA, 2003a)). The EPACMTP model includes a database of soil characteristics for each of three default soil types; residual water content is one of the soil characteristics included in these default databases. A statistical summary of the values used for each of the three default soil types, including the residual water content of the soil, is shown in Table 5.4. The cumulative frequency distribution of soil hydraulic conductivity values listed in Table 5.9 was generated by performing a default nationwide landfill modeling analysis using the regional site-based modeling methodology. For a given percentile (%) frequency and value pair in Table 5.9, the percentile denotes the relative frequency or likelihood of parameter values in the entire distribution being less than or equal to the corresponding parameter value in the right hand column.

Table 5.9 Cumulative Frequency Distribution of Residual Water Content

%	Residual Water Content (unitless)
0	1.06E-02
10	4.89E-02
25	6.09E-02
50	7.46E-02
75	8.57E-02
80	8.80E-02
85	9.07E-02
90	9.37E-02
95	9.81E-02
100	1.15E-01

Data Sources

The databases of soil characteristics for the three default soil types (which include the residual water content) were derived from soil hydraulic property data reported by Carsel and Parrish (1988).

Use In EPACMTP

The residual water content is an input to the unsaturated zone flow module and is used to calculate the moisture content in the soil under a given rate of leachate infiltration from the WMU.

5.2.3.5 Saturated Water Content (θ_s)

Definition

At atmospheric pressure, the saturated water content represents the maximum fraction of the total volume of soil that is occupied by the water contained in the soil.

Parameter Value or Distribution of Values

If site-specific data are available, then the saturated water content of the soil can be specified in the input file as a constant value or an empirical or statistical distribution of values.

Lacking site-specific data, a default distribution of soil hydraulic conductivity values may be used as part of the regional site-based modeling methodology (see Section 5.5 of the *EPACMTP Technical Background Document* (U.S. EPA, 2003a)). The EPACMTP model includes a database of soil characteristics for each of three default soil types; saturated water content is one of the soil characteristics included in these default databases. A statistical summary of the values used for each of the three default soil types, including the saturated water content of the soil, is shown in Table 5.4. The cumulative frequency distribution of soil hydraulic conductivity values listed in Table 5.10 was generated by performing a default nationwide landfill modeling analysis using the regional site-based modeling. For a given percentile (%) frequency and value pair in Table 5.10, the percentile denotes the relative frequency or likelihood of parameter values in the entire distribution being less than or equal to the corresponding parameter value in the right hand column.

Table 5.10 Cumulative Frequency Distribution of Saturated Water Content

%	Saturated Water Content (unitless)
0	4.10E-01
10	4.10E-01
25	4.30E-01
50	4.50E-01
75	4.50E-01
80	4.50E-01
85	4.50E-01
90	4.50E-01
95	4.50E-01
100	4.50E-01

Data Sources

The databases of soil characteristics for the three default soil types (which include the saturated water content) were derived from soil hydraulic property data reported by Carsel and Parrish (1988).

Use In EPACMTP

The saturated water content is an input to the unsaturated zone flow module and is used to calculate the moisture content in the soil under a given rate of leachate infiltration from the WMU.

5.2.3.6 Soil Bulk Density (ρ_b)**Definition**

The dry bulk density of the soil is the ratio of the mass of the solid soil to its total volume.

Parameter Value or Distribution of Values

If site-specific data are available, then the soil bulk density can be specified in the input file as a constant value or an empirical or statistical distribution of values.

Lacking site-specific data, a default distribution of soil hydraulic conductivity values may be used as part of the regional site-based modeling methodology (see Section 5.5 of the *EPACMTP Technical Background Document* (U.S. EPA, 2003a)). The EPACMTP model includes a database of soil characteristics for each of three default soil types; soil bulk density is one of the soil characteristics included in these default databases. A statistical summary of the values used for each of the three default soil types, including the soil bulk density, is shown in Table 5.4. The cumulative frequency distribution of soil hydraulic conductivity values listed in Table 5.11 was generated by performing a default nationwide landfill modeling analysis using the regional site-based modeling methodology. For a given percentile (%) frequency and value pair in Table 5.11, the percentile denotes the relative frequency or likelihood of parameter values in the entire distribution being less than or equal to the corresponding parameter value in the right hand column.

Table 5.11 Cumulative Frequency Distribution of Soil Bulk Density

%	Soil Bulk Density (g/cm³)
0	1.60E+00
10	1.60E+00
25	1.65E+00
50	1.65E+00
75	1.67E+00
80	1.67E+00
85	1.67E+00
90	1.67E+00
95	1.67E+00
100	1.67E+00

Data Sources

The databases of soil characteristics for the three default soil types (which include the bulk density) were derived from soil property data reported by Carsel et al (1988).

Use In EPACMTP

The dry soil bulk density (mass of soil per unit volume) is used to calculate the retardation coefficient of organic constituents and to convert soil mass to volume.

5.2.3.7 Percent Organic Matter (%OM)**Definition**

The percent organic matter is a measure of the organic material that is present within the soil of the unsaturated zone, measured as a weight percent.

Parameter Value or Distribution of Values

If site-specific data are available, then the percent organic matter in the soil can be specified in the input file as a constant value or an empirical or statistical distribution of values.

Lacking site-specific data, a default distribution of soil hydraulic conductivity values may be used as part of the regional site-based modeling methodology (see Section 5.5 of the *EPACMTP Technical Background Document* (U.S. EPA, 2003a)). The EPACMTP model includes a database of soil characteristics for each of three default soil types; hydraulic conductivity is one of the soil characteristics included in these default databases. A statistical summary of the values used for each of the three default soil types, including the percent organic matter in the soil, is shown in Table 5.4. The cumulative frequency distribution of soil hydraulic conductivity values listed in Table

5.12 was generated by performing a default nationwide landfill modeling analysis using the regional site-based modeling methodology. For a given percentile (%) frequency and value pair in Table 5.12, the percentile denotes the relative frequency or likelihood of parameter values in the entire distribution being less than or equal to the corresponding parameter value in the right hand column.

Table 5.12 Cumulative Frequency Distribution of Percent Organic Matter

%	Percent Organic Matter (unitless)
0	3.58E-03
10	1.05E-01
25	7.87E-02
50	4.05E-02
75	1.18E-01
80	1.42E-01
85	1.72E-01
90	2.15E-01
95	2.96E-01
100	1.69E+00

Data Sources

The databases of soil characteristics for the three default soil types (which include the percent organic matter) were derived from soil property data reported by Carsel et al (1988).

Use In EPACMTP

For organic constituents, the percent organic matter in the soil which is specified in the input file is internally converted by the EPACMTP model to fractional organic carbon content through the following equation (Enfield et al., 1982):

$$f_{oc} = \% OM / 174 \quad (5.1)$$

where:

f_{oc} = fractional organic carbon content,
 $\%OM$ = percent organic matter, and
 174 = conversion factor.

Once the fractional organic carbon content is obtained, it is used to calculate the unsaturated zone linear distribution coefficient for organic constituents (k_d , see Section 5.2.8) assuming that hydrophobic binding dominates the sorption process

(Karickhoff, 1985). The distribution coefficient is then used to calculate the amount by which contaminant transport is retarded relative to the ambient ground-water flow velocity within the vadose zone.

This input is not used for modeling the transport of metals.

5.2.4 **Unsaturated Zone Longitudinal Dispersivity (α_{Lu})**

Definition

Dispersion is the phenomenon by which a dissolved constituent in soil or ground water is mixed with uncontaminated water and becomes reduced in concentration at the perimeter of the plume. Not all of a constituent is traveling at the same velocity, due to differences in pore size and flow path length and friction along pore walls, resulting in mixing along the flow path which decreases solute concentrations. Note that the unsaturated zone longitudinal dispersivity is measured along the path of flow, that is, in the downward direction.

Parameter Value or Distribution of Values

The longitudinal dispersivity of the soil can be input as a constant value or a distribution of values, if site-specific data are available. If not, the dispersivity can be derived as a linear function of the total depth of the unsaturated zone according the following equation which is based on a regression analysis of data presented by EPRI (1985):

$$\alpha_{Lu} = 0.02 + 0.022 D_u \quad (5.2)$$

where

$$\begin{aligned} \alpha_{Lu} &= \text{longitudinal dispersivity (m)} \\ D_u &= \text{total depth of the unsaturated zone (m)} \end{aligned}$$

The cumulative frequency distribution of soil hydraulic conductivity values listed in Table 5.13 was generated by performing a default nationwide landfill modeling analysis using the regional site-based modeling methodology. The unsaturated zone dispersivity was specified as a derived variable in the input file, and this distribution of values was created through the Monte Carlo sampling of unsaturated zone thickness from the linked WMU site and HGDB databases (see Section 5.3.4). For a given percentile (%) frequency and value pair in Table 5.13, the percentile denotes the relative frequency or likelihood of parameter values in the entire distribution being less than or equal to the corresponding parameter value in the right hand column.

Table 5.13 Cumulative Frequency Distribution of Dispersivity

%	Dispersivity (m)
0	2.67E-02
10	5.70E-02
25	1.07E-01
50	1.54E-01
75	3.54E-01
80	4.23E-01
85	6.65E-01
90	9.59E-01
95	1.00E+00
100	1.00E+00

Data Sources

Lacking site-specific data to input, Equation 5.1 is used to calculate the unsaturated zone dispersivity. This equation is based on a regression analysis of data presented by EPRI (1985) (shown in Table 5.14) and has a correlation coefficient of 0.66.

Use In EPACMTP

The longitudinal dispersivity of the unsaturated zone is an input to the unsaturated zone transport module and is used to calculate the concentration history (breakthrough curve) of the constituent plume arriving at the water table.

Table 5.14 Compilation of field dispersivity values (EPRI, 1985)

Author	Type of Experiment	Vertical Scale of Experiment (m)	Longitudinal Dispersivity α_L (m)
Yule and Gardner (1978)	Laboratory	0.23	0.0022
Hildebrand and Himmelblau (1977)	Laboratory	0.79	0.0018
Kirda et al. (1973)	Laboratory	0.60	0.004
Gaudet et al. (1977)	Laboratory	0.94	0.01
Brissaud et al. (1983)	Field	1.00	0.0011, 0.002
Warrick et al. (1971)	Field	1.20	0.027
Van de Pol et al. (1977)	Field	1.50	0.0941
Biggar and Nielsen (1976)	Field	1.83	0.05
Kies (1981)	Field	2.00	0.168
Jury et al. (1982)	Field	2.00	0.0945
Andersen et al. (1968)	Field	20.00	0.70
Oakes (1977)	Field	20.00	0.20

5.2.5 Freundlich Adsorption Isotherm Parameters

An adsorption isotherm is an expression of the equilibrium relationship between the aqueous concentration and the sorbed concentration of a chemical constituent (organic or metal) at a constant temperature. One of the general models of the sorption process is the Freundlich isotherm, defined as follows:

$$S = KC^\eta \quad (5.3a)$$

where:

- S = mass of constituent that is sorbed per dry unit weight of solid (mg/kg)
- K = Leading coefficient of the Freundlich isotherm (mg/kg)/(mg/L) $^\eta$
- C = aqueous concentration of the constituent at equilibrium with the sorbed mass (mg/L)
- η = Freundlich isotherm exponent (dimensionless)

If the sorptive behavior of a constituent can be described by the Freundlich isotherm, then when $\log C$ is plotted against $\log S$, the resulting relationship will be linear with a slope of η and an intercept of $\log K$. A special case is when η is equal to 1.0. In this case, the sorption isotherm is linear and the leading Freundlich coefficient is known as the linear solid-liquid phase distribution coefficient (K_d). A linear isotherm is commonly used to describe the subsurface fate and transport of organic constituents, assuming that hydrophobic binding dominates the sorption process (Karickhoff, 1985). In this case, the K_d can be calculated as follows:

$$K_d = k_{oc} f_{oc} \quad (5.3b)$$

where

K_d	=	leading Freundlich coefficient (distribution coefficient) (cm^3/g)
k_{oc}	=	normalized organic carbon distribution coefficient (cm^3/g)
f_{oc}	=	fractional organic carbon content (dimensionless)

Equation (5.3a) may be recast as:

$$S = (KC^{\eta-1})C = K_d(C)C \quad (5.3c)$$

where:

S	=	mass of constituent that is sorbed per dry unit weight of solid (mg/kg)
K	=	Leading coefficient of the Freundlich isotherm ($\text{mg}/\text{kg})/(\text{mg}/\text{L})^\eta$
C	=	aqueous concentration of the constituent at equilibrium with the sorbed mass (mg/L)
η	=	Freundlich isotherm exponent (dimensionless)
K_d	=	distribution coefficient (cm^3/g)

The distribution coefficient, K_d , in Equation 5.3c is non-linear and is a function of aqueous concentration. In EPACMTP, the non-linear K_d function in Equation (5.3c) may be more general than the Freundlich type (see Section 5.2.5.1) below.

To model the fate and transport of constituents with EPACMTP, the user must specify two adsorption isotherm parameters: the Freundlich sorption coefficient (K or K_d) and the Freundlich exponent (η). These two parameters are described in Sections 5.2.5.1 and 5.2.5.2, below.

5.2.5.1 Leading Coefficient of Freundlich Isotherm for Unsaturated Zone (K or K_d)

Definition

The leading coefficient of the Freundlich isotherm is a constant used to describe the sorptive behavior of a constituent. When the sorption data are plotted as $\log C$ versus $\log S$, the intercept of the resulting line is equal to $\log K$. In the special case of a linear isotherm, the leading Freundlich coefficient is known as the linear solid-liquid phase distribution coefficient (K_d) (commonly called the distribution coefficient).

Parameter Value or Distribution of Values

When modeling organic constituents with EPACMTP, the leading Freundlich coefficient is generally specified as a derived parameter in the input file. If derived, the leading Freundlich coefficient (K_d) is automatically assumed linear and calculated by the model according to Equation 5.3b. In this case, f_{oc} is internally calculated from the percent organic matter specified in the unsaturated zone-specific input group according to Equation 5.2, and k_{oc} is a constituent-specific input value (see Section 3 of this document). However, if site-specific data are available, a constant value or distribution of values could be used for the leading Freundlich coefficient.

When modeling metals transport in the unsaturated zone with EPACMTP, the leading Freundlich coefficient can be specified as a constant value or as a distribution of values, based either on site-specific data or adsorption data reported in the scientific literature. Alternatively, tables of non-linear sorption isotherms developed using the MINTEQA2 geochemical model, or equations comprising pH -based (linear) isotherms can be used. For the latter two cases (non-linear isotherms or pH -based linear isotherms) this input parameter is not used; the record in the input file is ignored by the model. Instead, the non-linear K_d (Equation 5.3c) is either provided in tabular form as a function of the concentration value or calculated as a function of pH (see Sections 3.3.3.2 and 3.3.3.1.2, respectively).

Data Sources

Generally, the K_d for organic constituents is specified as a derived parameter; however, if this option is not appropriate and site-specific data are not available, there are studies in the scientific literature that provide compilations of K_d 's that have been measured in the field (for instance, see *Risk Assessment for the Listing Determinations for Inorganic Chemical Manufacturing Wastes*; U.S. EPA, 2000). In this case, the leading Freundlich coefficient would be specified as either a constant value or a distribution of values (and the Freundlich exponent would be set to its default value of 1.0).

The leading Freundlich coefficient for metals is specified using either the non-linear MINTEQA2 isotherms or pH -based linear isotherms that were developed specifically for use with the EPACMTP model (see Section 3.3.3). However, if

neither of these two options is appropriate and site-specific data are not available, there are studies in the scientific literature that provide compilations of K_d 's that have been measured in the field (for instance, see Appendix I of U.S. EPA, 2000). In this case, the leading Freundlich coefficient would be specified as either a constant value or a distribution of values.

Use In EPACMTP

The leading Freundlich coefficient (also called the distribution coefficient) is one of the parameters used to calculate the amount by which contaminant transport is retarded relative to the ambient ground-water flow velocity within the unsaturated zone. It is an input to the unsaturated zone transport module. For organic constituents that are subject to hydrolysis, this input is also used as a parameter to calculate the overall hydrolysis rate.

5.2.5.2 Exponent of Freundlich Isotherm for Unsaturated Zone (n)

Definition

The exponent of the Freundlich isotherm is a constant used to describe the sorptive behavior of a constituent. When the sorption data are plotted as $\log C$ versus $\log S$, the slope of the resulting line is equal to n . In the special case of a linear isotherm, the exponent of the Freundlich isotherm is equal to 1.0.

Parameter Value or Distribution of Values

For modeling organic constituents, the default value of the Freundlich exponent is 1.0, meaning a linear adsorption isotherm is used.

Generally, the distribution coefficient for metals is specified using either tabulated non-linear MINTEQA2 isotherms or pH-based linear isotherms that were developed specifically for use with the EPACMTP model (see Section 3.3.3). In these two cases, the K_d data is read in from an auxiliary input file or internally calculated, and the Freundlich isotherm coefficient and exponent are not used. If the leading Freundlich coefficient is specified using an empirical distribution of values (e.g., based on reported K_d values in the scientific literature), then the Freundlich isotherm exponent should be set equal to 1.0.

If this parameter is omitted from the data file, it is assigned a default value of 1.0, which is equivalent to specifying a linear sorption isotherm.

In EPACMTP Version 2.0, only the case of $n = 1$ is permitted. Non-linear isotherms (see Equation 5.3c) are handled using the tabular type of input described in Section 3.3.3.2.

Data Sources

For modeling organic constituents, the Freundlich isotherm exponent is generally set to its default value of 1.0, and so no specific data source is used to determine the appropriate value for the Freundlich exponent.

For modeling metal constituents, the Freundlich isotherm exponent is not used as an input parameter, and so no specific data source is used (see Section 3.3.3.2). If literature or site-specific data are used to specify a non-linear adsorption isotherm, modeling of the adsorption process is implemented via tabular input describing the relationship in Equation 5.3c.

Use In EPACMTP

The Freundlich exponent is one of the parameters used to calculate the amount by which contaminant transport is retarded relative to the ambient groundwater flow velocity within the unsaturated zone; it is an input to the unsaturated zone transport module.

5.2.6 Chemical Degradation Rate Coefficient for Unsaturated Zone (λ_{cu})**Definition**

EPACMTP accounts for all transformation processes (both biological and chemical) using a lumped first-order decay coefficient. This overall decay coefficient is the sum of the chemical and biological transformation coefficients. The chemical degradation coefficient for the unsaturated zone is simply the rate of decay that is caused by chemical (usually hydrolysis) reactions in the unsaturated zone.

Parameter Value or Distribution of Values

By default, the chemical degradation coefficient in the unsaturated zone is set to be internally derived using the hydrolysis rate constants and the unsaturated zone properties according to Equation 3.4. However, if site-specific data are available, this parameter can be specified as a constant value or a distribution of values. In this case, the hydrolysis rate constants can be omitted from the input file.

Data Sources

If this parameter is not derived by the model, then a site-specific data source must be used to determine the appropriate input value.

Use In EPACMTP

The chemical degradation coefficient is used by the model to calculate the amount by which contaminant concentrations within the vadose zone are attenuated due to chemical hydrolysis; it is an input to the unsaturated zone transport module and is one of the parameters required to solve the transport equation for dissolved

leachate constituents (see Sections 3.3.4 and 4.4.4 of the *EPACMTP Technical Background Document* (U.S. EPA, 2003a).

5.2.7 Biodegradation Rate Coefficient for Unsaturated Zone (λ_{bu})

Definition

EPACMTP accounts for all transformation processes (both biological and chemical) using a lumped first-order decay coefficient. This overall decay coefficient is the sum of the chemical and biological transformation coefficients. The biological degradation coefficient for the unsaturated zone is simply the rate of decay that is caused by biological processes in the unsaturated zone.

Parameter Value or Distribution of Values

By default, the biological degradation coefficient in the unsaturated zone is set equal to zero. However, if site-specific data are available, this parameter can be specified as a constant value or a distribution of values.

Data Sources

If the input value of this parameter is non-zero, then a site-specific data source must be used to determine the appropriate input value.

Use In EPACMTP

The biological degradation coefficient is used by the model to calculate the amount by which contaminant concentrations within the vadose zone are attenuated due to biological processes; it is an input to the unsaturated zone transport module and is one of the parameters required to solve the transport equation for dissolved leachate constituents (see Sections 3.3.4 and 4.4.4 of the *EPACMTP Technical Background Document* (U.S. EPA, 2003a).

5.2.8 Soil Temperature (T)

Definition

The soil temperature is the long-term average temperature within the vadose zone. Note that although the temperature within the vadose zone is not an explicit model input, this temperature is assumed by EPACMTP to be the same as that of the aquifer.

Parameter Value or Distribution of Values

As modeled in EPACMTP, soil temperature affects the transformation rate of constituents that are subject to hydrolysis, through the effect of temperature on reaction rates (see Section 3.3.2.2). In the development of the site data files for each WMU type, information on average annual temperatures in shallow ground-

water systems (Todd, 1980) were used to assign a temperature value to each WMU in the modeling database, based on the unit's geographical location. For each WMU site, the assigned temperature was an average of the upper and lower values for that temperature region, as shown in Figure 5.1. In other words, all WMU's located in the band between 10° and 15° were assigned a temperature value of 12.5 °C.

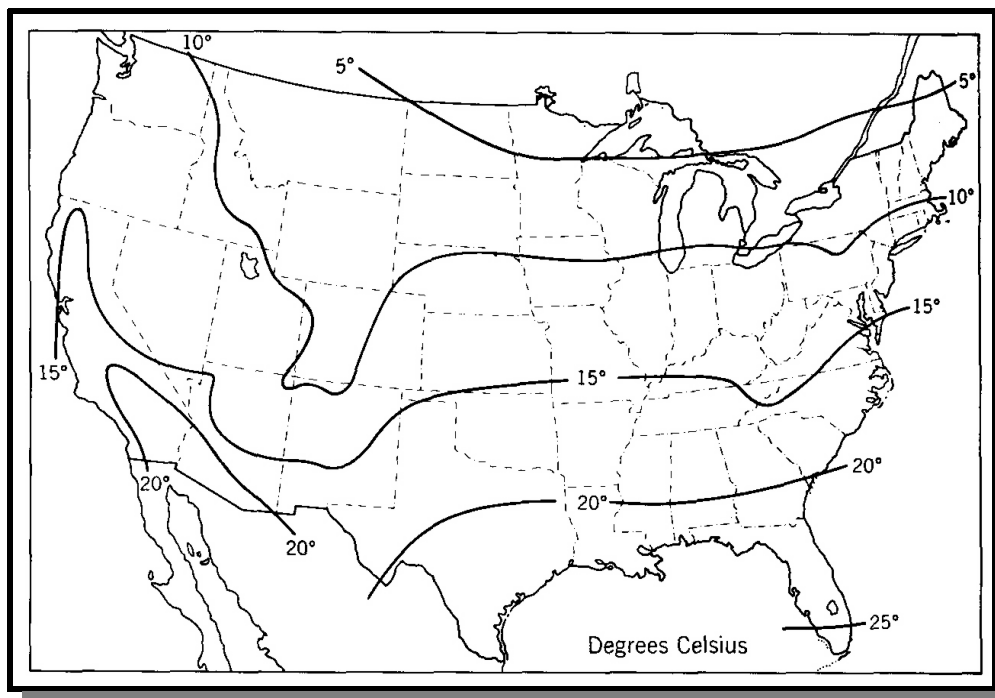


Figure 5.1 Ground-water Temperature Distribution for Shallow Aquifers in the United States (from Todd, 1980)

Data Sources

Information on average annual temperatures in shallow ground-water systems from Todd (1980) were used to assign a temperature value to each WMU site in the site data files, based on the unit's geographical location.

Use In EPACMTP

When the EPACMTP model is run using the regional, site-based methodology, for each Monte Carlo realization, the model selects a site, at random, from those in the site data file. Since the original data sets did not include all the site-related input files required by the EPACMTP model, other data sources, such as this map of ground-water temperatures, are utilized to create a complete data set. For each WMU site, the ground-water temperature was assigned using the data from Todd (1980) and the unit's geographical location.

In a location-adjusted modeling analysis, a site-specific ground-water temperature can be directly specified in the input file – either as a constant value or as a statistical or empirical distribution of values.

The aquifer temperature associated with the modeled site and the specified hydrolysis rate constants are then used by the model to derive the appropriate temperature-dependent first-order hydrolysis rate for organic constituents. Note that although the temperature of the ground-water within the vadose zone is not an explicit model input, the EPACMTP model assumes that the soil temperature is the same as that of the aquifer.

5.2.9 Soil pH (pH)

pH is defined as the negative of the base-10 logarithm of the hydrogen ion $[H^+]$ concentration in solution. pH is a measure of acidity. pH values below 7 indicate acidic conditions; values above 7 indicate alkaline conditions.

Parameter Value or Distribution of Values

A nationwide ground-water pH distribution was derived from EPA's STORET database (U.S. EPA, 1996). EPACMTP assumes that the ground water is sufficiently buffered such that pH is not influenced by the input of contaminants or changes in temperature. The default distribution is an empirical distribution with a median value of 6.8 or lower and upper bounds of 3.2 and 9.7, respectively. Note that the value generated for the ground-water pH is assumed to apply to the unsaturated zone as well.

Data Sources

The pH data distribution was developed from nearly 25,000 field-measured pH values in EPA's STORET water quality database (U.S. EPA, 1996). EPA used these data to develop a pH distribution for ground water that is used in EPACMTP for the unsaturated zone as well.

Use In EPACMTP

pH is used in the calculation of hydrolysis rates for organic constituents, in accordance with Equation 3.6.

pH is also one of the key parameters that controls sorption and mobility of metal constituents. When the default, MINTEQA2 sorption isotherms are used in EPACMTP, pH is one of the key master variables that controls the selection of a particular isotherm for each model realization in the Monte Carlo simulation process.

5.3 SATURATED ZONE PARAMETERS

In the saturated zone, EPACMTP simulates ground-water flow and three-dimensional constituent transport from the water table to a downgradient well. The

saturated zone-specific inputs used by the model to simulate the fate of constituents as they are transported through the subsurface include particle diameter, porosity, bulk density, aquifer thickness, hydraulic conductivity, hydraulic gradient, anisotropy ratio, dispersivity, ground-water temperature and pH, and parameters describing the sorption and/or degradation of the modeled constituent. The primary model output is a prediction of the constituent concentration arriving at a downgradient well.

The primary source of data for the default distributions used in the saturated zone module is the Hydrogeologic Database for Ground-Water Modeling (HGDB), assembled by Rice University on behalf of the American Petroleum Institute (API) (Newell et al., 1990). This database provides probability distributions for the following three aquifer-specific inputs for various types of subsurface environments: aquifer thickness, hydraulic conductivity, and hydraulic gradient (data on the unsaturated zone thickness is also included in this database, but this parameter is discussed with the other unsaturated zone parameters in Section 5.2).

All of the saturated zone parameters are individually described in the following sections.

5.3.1 Particle Diameter (d)

Definition

The particle diameter is defined as the mean diameter of the particles constituting the aquifer materials.

Parameter Value or Distribution of Values

Lacking a site-specific value or distribution of values, this input value can be specified using a default distribution of values (the default option) or it can be derived based on the aquifer's porosity. The default distribution of values was created from data compiled by Shea (1974) and is presented below in Table 5.15. For a given percentile (%) frequency and value pair in this table, the percentile denotes the relative frequency or likelihood of parameter values in the entire distribution being less than or equal to the corresponding parameter value in the right hand column.

Table 5.16 lists the cumulative frequency distribution of particle diameter that is generated in a default landfill modeling analysis using the regional site-based modeling methodology. For a given percentile (%) frequency and value pair in Table 5.16, the percentile denotes the relative frequency or likelihood of parameter values in the entire distribution being less than or equal to the corresponding parameter value in the right hand column.

Table 5.15 Empirical distribution of mean particle diameter (based on Shea, 1974)

Cumulative Probability	Particle Diameter (cm)
3.9×10^{-4}	0.000
7.8×10^{-4}	0.038
1.6×10^{-3}	0.104
3.1×10^{-3}	0.171
6.3×10^{-3}	0.262
1.25×10^{-2}	0.371
2.5×10^{-2}	0.560
5.0×10^{-2}	0.792
1.0×10^{-1}	0.904
2.0×10^{-1}	0.944
4.0×10^{-1}	0.976
8.0×10^{-1}	1.000

Table 5.16 Cumulative Frequency Distribution of Particle Diameter

%	Particle Diameter (cm)
0	4.00E-04
10	1.50E-03
25	5.57E-03
50	1.91E-02
75	4.09E-02
80	4.60E-02
85	5.56E-02
90	7.62E-02
95	9.73E-02
100	2.11E-01

Alternatively, if the particle diameter is treated as a derived parameter, then its value is calculated using the value of porosity (which may be constant or randomly generated from a probability distribution) using the following empirical relationship based on data reported by Davis (1969):

$$d = \exp [0.261 - \phi\gamma 0.0385] \quad (5.4)$$

where:

- d = mean particle diameter (cm)
- ϕ = total porosity (dimensionless)
- γ = van Genuchten soil-specific shape parameter (dimensionless)

Data Sources

For Monte Carlo analyses, an empirical distribution of values is typically used for the mean particle diameter. This distribution of values is based on data compiled by Shea (1974) in which a frequency distribution of particle sizes is presented that is based on analysis of 11,000 samples.

Alternatively, if the particle diameter is treated as a derived parameter, then its value is calculated from the porosity using Equation 5.4 based on data reported by Davis (1969).

Use In EPACMTP

For Monte Carlo analyses, the mean particle diameter is typically used to calculate porosity and bulk density of the aquifer materials. Bulk density is an input to the saturated zone flow and transport modules. In the transport module, it is one of several parameters used to calculate the degree to which contaminant velocities are retarded relative to the ambient ground-water flow velocity within the aquifer.

5.3.2 Porosity (ϕ)

Definition

Porosity is the ratio of the volume of void spaces in rock or sediment to the total volume of rock or sediment. For contaminant transport modeling, it is more appropriate to use effective porosity, ϕ_e , than total porosity. The effective porosity can be significantly smaller than the total porosity. However, the EPACMTP input parameter porosity can represent either total or effective porosity, depending upon how it is specified, as described below.

Parameter Value or Distribution of Values

Lacking a site-specific value or distribution of values, this input value can be calculated based on the aquifer's particle diameter by rewriting Equation 5.4 to solve for porosity, as shown below:

$$\phi = 0.261 - 0.0385 \ln(d) \quad (5.5)$$

where:

$$\begin{array}{ll} d & = \text{mean particle diameter (cm)} \\ \phi & = \text{total porosity (dimensionless)} \end{array}$$

Equation 5.5 yields the total porosity of the aquifer, but for contaminant transport modeling, it is more appropriate to use effective porosity, ϕ_e , than total porosity. The effective porosity can be significantly smaller than the total porosity, although a constant relationship between these two parameters cannot be established. McWorter and Sunada (1977) present data on total and effective porosity for a range of aquifer materials. Their data was used to create a default methodology whereby the EPACMTP model calculates the effective porosity based on the total porosity and the grain size (see Table 5.17).

For Monte Carlo assessments, the effective porosity of the aquifer is, by default, specified as a derived parameter in the EPACMTP input file. In this case, the model assumes that the actual ratio between effective and total porosity varies uniformly between the upper and lower value for ϕ_e/ϕ in each particle-size class for a given value of the mean aquifer grain size class. For a given value of the mean aquifer grain size, the total porosity can thus be converted into effective porosity.

Please note that EPACMTP makes the conversion from total of effective porosity only if porosity is specified as a derived parameter (porosity is calculated from grain size), the default setting in the input file. In all other cases, no conversion is performed and the user must specify the actual porosity data to be used by the model, providing a constant value or distribution of values for either total porosity or effective porosity directly.

Table 5.17 Ratio between effective and total porosity as a function of particle diameter (after McWorter and Sunada, 1977)

Mean Particle Diameter (cm)	ϕ_e/ϕ Range
$\leq 6.25 \cdot 10^{-3}$	0.03 - 0.77
$6.25 \cdot 10^{-3} - 2.5 \cdot 10^{-2}$	0.04 - 0.87
$2.5 \cdot 10^{-2} - 5.0 \cdot 10^{-2}$	0.31 - 0.91
$5.0 \cdot 10^{-2} - 1.0 \cdot 10^{-1}$	0.58 - 0.94
$> 1.0 \cdot 10^{-1}$	0.52 - 0.95

Data Sources

If the porosity is treated as a derived parameter (the default setting), then the total porosity is calculated from the mean particle diameter using Equation 5.5 which is based on data reported by Davis (1969). The total porosity is then converted to effective porosity by randomly choosing a ratio between effective and total porosity; this conversion is accomplished through the use of ranges of values for the ratio between effective and total porosity as a function of mean particle diameter that are derived from data presented in McWorter and Sunada (1977).

Use In EPACMTP

For Monte Carlo analyses, the porosity, whether directly input or derived, is used to calculate the bulk density of the aquifer materials. Bulk density is an input to the saturated zone flow and transport modules. In the saturated zone flow module, bulk density is used in the calculation of the ground-water seepage velocity. In the transport module, bulk density is one of several parameters used to calculate the degree to which contaminant velocities are retarded relative to the ambient ground-water flow velocity within the aquifer.

5.3.3 Bulk Density (ρ_b)**Definition**

Bulk density is defined as the mass of aquifer solid material per unit volume of the aquifer, in g/cm³ or mg/L. Bulk density takes into account the fraction of the volume that is taken up by pore space.

Parameter Value or Distribution of Values

Lacking site-specific data for bulk density, this input can be derived from the porosity of the aquifer. Assuming the particle density to be 2.65 g/cm³, the bulk density can be calculated using the following equation from Freeze and Cherry (1979):

$$\rho = 2.85 (1 - \phi) \quad (5.6)$$

where

ρ_b = bulk density of the soil (g/cm³).

ϕ = total porosity of the aquifer material (dimensionless)

Table 5.18 lists the cumulative frequency distribution of bulk density that is generated in a default landfill modeling analysis using the regional site-based modeling methodology. For a given percentile (%) frequency and value pair in Table 5.18, the percentile denotes the relative frequency or likelihood of parameter values in the entire distribution being less than or equal to the corresponding parameter value in the right hand column.

Table 5.18 Cumulative Frequency Distribution of Bulk Density

%	Soil Bulk Density (g/cm ³)
0	1.16E+00
10	1.30E+00
25	1.43E+00
50	1.56E+00
75	1.63E+00
80	1.64E+00
85	1.66E+00
90	1.70E+00
95	1.72E+00
100	1.80E+00

Data Sources

In the absence of a site specific value or distribution of values for bulk density, this input can be specified as a derived parameter in the EPACMTP input file. In this case, the input value is calculated from the aquifer porosity by assuming the particle density to be 2.65 g/cm³ and using the relationship from Freeze and Cherry (1979) that is presented as Equation 5.6.

Use In EPACMTP

Bulk density is an input to the saturated zone flow and transport modules. In the saturated zone flow submodule, bulk density is used in the calculation of the ground-water seepage velocity. In the transport flow submodule, bulk density is one of several parameters used to calculate the degree to which contaminant velocities are retarded relative to the ambient ground-water flow velocity within the aquifer.

5.3.4 Aquifer Characteristics

In the absence of site-specific data to input, default distributions of correlated values can be used in EPACMTP for the following aquifer characteristics:

1. Depth to ground water;
2. Saturated zone thickness;
3. Saturated zone hydraulic conductivity; and
4. Saturated zone hydraulic gradient.

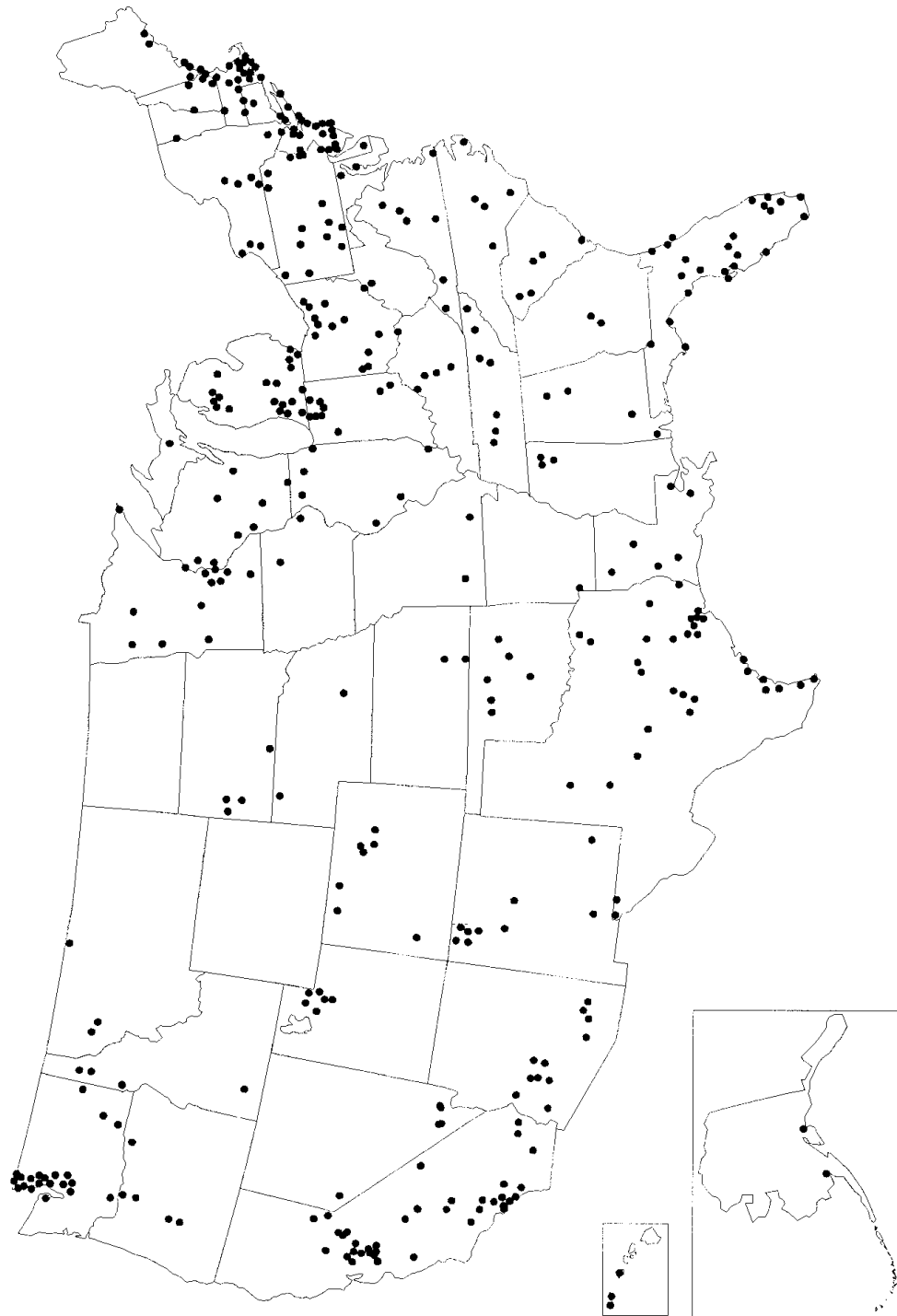
These default distributions are derived from the Hydrogeologic Database for Ground-Water Modeling (HGDB), assembled by Rice University on behalf of the American Petroleum Institute (API) (Newell et al., 1990). The data in this hydrogeological database were collected by independent investigators for approximately 400 hazardous waste sites throughout the United States; the geographical locations of these sites are shown in Figure 5.2 (p. 5-37). In the HGDB, the data are grouped into twelve subsurface environments, which are based on EPA's DRASTIC classification of hydrogeologic settings (U.S. EPA, 1985). Table 5.19 lists these hydrogeologic environments, and a brief description of each environment is presented in Section 5.3.4.2. Table 5.19 includes a total of 13 categories; 12 are distinct subsurface environments, while the 13th category, which is labeled "other" or "unknown", was used for waste sites that could not be classified into one of the first 12 environments. The subsurface parameter values in this 13th category are simply averages of the parameter values in the 12 actual subsurface environments. The resulting database of aquifer types, with each aquifer type consisting of an empirical distribution of values for each of the four aquifer parameters, is presented in its entirety in Appendix D.

Table 5.19 HGDB Hydrogeologic Environments (from Newell et al., 1990)

Region	Description
1	Metamorphic and Igneous
2	Bedded Sedimentary Rock
3	Till Over Sedimentary Rock
4	Sand and Gravel
5	Alluvial Basins Valleys and Fans
6	River Valleys and Flood Plains with Overbank Deposits
7	River Valleys and Flood Plains without Overbank
8	Deposits
9	Outwash
10	Till and Till Over Outwash
11	Unconsolidated and Semi-consolidated Shallow
12	Aquifers
13	Coastal Beaches
	Solution Limestone
	Other (Not classifiable)

The key feature of this database is that it provides a set of correlated values of the four parameters for each of the 400 sites in the database. That is, the value of each parameter is associated with the three other subsurface parameters reported for the same site. The regional site-based modeling methodology in EPACMTP preserves these correlations because having information on some parameters allows us to develop more accurate estimates for missing parameter values. As described in Section 5.5 of the *EPACMTP Technical Background Document* (U.S. EPA, 2003a), the regional site-based modeling methodology is an attempt to ensure that the combination of parameter values that are randomly generated by the Monte Carlo module of EPACMTP represents a realistic set of site conditions. This methodology is called 'regional site-based' because waste site databases are linked by each site's geographic location and underlying aquifer type to regional databases of climatic and subsurface parameters, respectively. In this way, the regional site-based approach attempts to approximate the ideal situation where we have a complete set of the site-specific input data required to run the EPACMTP model for each waste site in a statistically valid subset of the universe of waste management units in the United States.

In developing the regional site-based modeling methodology in EPACMTP, the U.S. EPA used the HGDB in conjunction with a geographical classification of aquifers developed by the United States Geological Survey (Heath, 1984) to assign each waste site in our nationwide database of Subtitle D WMU's (see Section 2.2) to one of the 13 subsurface environments included in the HGDB. For each type of WMU, we used information on its location (see Figures 2.2 - 2.5), in combination with USGS state-by-state aquifer maps to determine the type of subsurface environment at that site. Sites that could not be classified into one of the 12 categories were assigned as "other" (that is, they were assigned to environment number 13). The regional site-based modeling methodology in EPACMTP is then used to assign a probability distribution of hydrogeologic parameter values to each WMU location. This methodology is consistent with the methodology used to assign HELP-derived infiltration and recharge rates to each waste site in our nationwide database of Subtitle D WMU's (see Section 4.2 and Appendix A).



**Figure 5.2 Geographical distribution of sites in the API-HGDB data base
(Reproduced from API, 1989)**

5.3.4.1 **Methodology**

Fundamentally, the approach used for a site-based Monte Carlo analysis consists of conducting the modeling analysis for the existing sites in our nationwide database of Subtitle D WMU's (see Section 2.2) on the assumption that these sites are an adequate representation of the universe of possible waste sites in the U.S. Since the original data sets (derived from the *1986 Subtitle D Survey* (U.S. EPA, 1986) and the *Surface Impoundment Study* (U.S. EPA, 2001a) only include the area, volume, location and relative weight of the facility, other data sources were utilized to determine the additional input parameters required by the EPACMTP model.

As summarized above, the ground-water parameter values are generated using the existing WMU parameter databases (which assign each waste site to a climate region and a hydrogeologic environment) together with the HGDB database of hydrogeologic parameters and the databases of HELP-derived infiltration and recharge rates. These databases are all included in an auxiliary input file called the site data file. The following is a description of how the regional, site-based modeling methodology is used to generate these hydrogeologic parameter values during the course of a typical Monte Carlo analysis for nationwide assessment purposes:

- For each Monte Carlo realization, EPACMTP selects a WMU site, at random, from the database of WMU sites. The original databases of WMU sites from which the data in the site data file were compiled included the facility location, area and volume. The EPACMTP model samples the sites in the site data files with replacement, i.e., the same site may be selected more than once. The probability of selecting a specific site depends on the relative weight assigned to that site in the original survey. Note that even if the same site is sampled more than once during the course of a Monte Carlo analysis in EPACMTP, the specific values of infiltration rate, hydrogeologic parameters, and receptor well location will still vary; likewise, the resulting receptor well concentration value will change, as well.
- Given the waste site's geographic location, the climatic region in which the site is located was identified and added to the WMU site database in the EPACMTP site data file. For landfills, waste piles, and land application units, the climatic region, the generated soil type, and the liner design (if any) are then used by the model to determine the infiltration rate of the site. In the no-liner and single-clay liner scenarios, these infiltration rates are determined using the database of rates generated with the HELP water balance model. For the composite liner scenario, these infiltration rates are internally calculated by the model using the relationships described in Sections 4.3.1 and 4.3.2. For surface impoundments (all liner scenarios), the infiltration rates are internally calculated by the model using the relationships described in Sections 4.3.4. For all WMU types, the climatic region and the generated soil type are used by the model to determine the ambient regional recharge rate of the site.

- Given the waste site's geographic location, the aquifer underlying the site was classified (using USGS state ground-water resources inventory maps) and added to the WMU site database in the EPACMTP site data file. The hydrogeologic parameters for the site are determined by selecting at random a set of aquifer characteristics (depth to ground water, aquifer thickness, hydraulic gradient, and hydraulic conductivity) from those available in the HGDB database for that hydrogeologic environment. In the case where the selected set of aquifer characteristics has missing values, a joint probability distribution (derived for each ground-water region) is used to generate the missing value as a function of the known values.
- The remaining parameters for the waste site (e.g., x, y and z coordinates of the receptor well) are generated according to their specifications in the input file. The ground-water flow and transport modules are then used to compute the resulting receptor well concentration for the site.
- These steps are then repeated for the desired number of iterations to yield a distribution of receptor well concentrations which represent the nationwide distribution of drinking water exposure concentrations. These modeling results can then be directly used in a forward risk calculation, or they can be post-processed to yield the ground-water dilution-attenuation factor (DAF) that can be used in a backward risk calculation to calculate an allowable threshold for the waste or leachate concentration.

5.3.4.2 Hydrogeologic Environment (IGWR)

Definition

The different hydrogeologic environments are represented in EPACMTP by means of a numerical index. The hydrogeologic environment index is simply a sequential number assigned to each hydrogeologic environment in the default database included with EPACMTP in order to provide a simple means of specifying which correlated set of aquifer characteristics should be used to model the given WMU site.

Parameter Value or Distribution of Values

To perform a standard Monte Carlo analysis using the regional site-based modeling methodology, the hydrogeologic environment index should be left in its default setting which will ensure that the appropriate climatic data is used for each WMU site in the database. However, if a location-adjusted or a quasi-site-specific analysis is being performed, then this input can either be omitted from the input file (if site-specific infiltration and recharge rates are available) or set to the appropriate

constant value to make use of the default set of aquifer characteristics which are included in the site data file.

The text boxes on the following pages provide a summary of the characteristics of each hydrogeologic environment.

Hydrogeologic Environment Descriptions

1) Igneous and Metamorphic Rocks

This hydrogeologic environment is underlain by consolidated bedrock of volcanic origin. This hydrogeologic environment setting is typically associated with steep slopes on the sides of mountains, and a thin soil cover. Igneous and metamorphic rocks generally have very low porosities and permeabilities. This hydrogeologic environment can occur throughout the United States, but is most prevalent in the western US.

2) Bedded Sedimentary Rock

Sedimentary rock is formed through erosion of bedrock. Deposited layers of eroded material may later be buried and compacted to form sedimentary rock. Generally, the deposition is not continuous but recurrent, and sheets of sediment representing separate events come to form distinct layers of sedimentary rock. Typically, these deposits are very permeable and yield large quantities of ground water. Examples of this hydrogeologic environment setting are found throughout the United States.

3) Till Over Sedimentary Rock

This hydrogeologic environment is found in glaciated regions in the northern United States which are frequently underlain by relatively flat-lying consolidated sedimentary bedrock consisting primarily of sandstone, shale, limestone, and dolomite. The bedrock is overlain by glacial deposits which consist chiefly of till, a dense unsorted mixture of soil and rock particles deposited directly by ice sheets. Ground water occurs both in the glacial deposits and in the sedimentary bedrock. Till deposits often have low permeability.

4) Sand and Gravel

Sediments are classified into three categories based upon their relative sizes; gravel, consisting of particles that individually may be boulders, cobbles or pebbles; sand, which may be very coarse, coarse, medium, fine or very fine; and mud, which may consist of clay and various size classes of silt. Sand and gravel hydrogeologic environments are very common throughout the United States and frequently overlie consolidated and semi-consolidated sedimentary rocks. Sand and gravel aquifers have very high permeabilities and yield large quantities of ground water.

5) Alluvial Basins, Valleys and Fans

Thick alluvial deposits in basins and valleys bordered by mountains typify this hydrogeologic environment. Alluvium is a general term for clay, silt, sand and gravel that was deposited during comparatively recent geologic time by a stream or other body of running water. The sediments are deposited in the bed of the stream or on its flood plain or delta, or in fan shaped deposits at the base of a mountain slope. Alluvial basins, valleys and fans frequently occupy a region extending from the Puget Sound-Willamette Valley area of Washington and Oregon to west Texas. This region consists of alternating basins or valleys and mountain ranges. The surrounding mountains, and the bedrock beneath the basins, consist of granite and metamorphic rocks. Ground water is obtained mostly from sand and gravel deposits within the alluvium. These deposits are interbedded with finer grained layers of silt and clay.

6) River Alluvium with Overbank Deposits

This hydrogeologic environment is characterized by low to moderate topography and thin to moderately thick sediments of flood-deposited alluvium along portions of a river valley. The alluvium is underlain by either unconsolidated sediments or fractured bedrock of sedimentary or igneous/metamorphic origin. Water is obtained from sand and gravel layers which are interbedded with finer grained alluvial deposits. The alluvium typically serves as a significant source of water. The flood plain is covered by varying thicknesses of fine-grained silt and clay, called overbank deposits. The overbank thickness is usually greater along major streams and thinner along minor streams but typically averages 5 to 10 feet.

Hydrogeologic Environment Descriptions (continued)**7) River Alluvium without Overbank Deposits**

This hydrogeologic environment is identical to the River Alluvium with Overbank Deposits environment except that no significant fine-grained flood plain deposits occupy the stream valley. The lack of fine grained deposits may result in significantly higher recharge in areas with ample precipitation.

8) Outwash

Sand and gravel removed or “washed out” from a glacier by streams is termed outwash. This hydrogeologic environment is characterized by moderate to low topography and varying thicknesses of outwash that overlie sequences of fractured bedrock of sedimentary, metamorphic or igneous origin. These sand and gravel outwash deposits typically serve as the principal aquifers within the area. The outwash also serves as a source of regional recharge to the underlying bedrock.

9) Till and Till Over Outwash

This hydrogeologic environment is characterized by low topography and outwash materials that are covered by varying thicknesses of glacial till. The till is principally unsorted sediment which may be interbedded with localized deposits of sand and gravel. Although ground water occurs in both the glacial till and in the underlying outwash, the outwash typically serves as the principal aquifer because the fine grained deposits have been removed by streams. The outwash is in direct hydraulic connection with the glacial till and the glacial till serves as a source of recharge for the underlying outwash.

10) Unconsolidated and Semi-consolidated Shallow Surficial Aquifers

This hydrogeologic environment is characterized by moderately low topographic relief and gently dipping, interbedded unconsolidated and semi-consolidated deposits which consist primarily of sand, silt and clay. Large quantities of water are obtained from the surficial sand and gravel deposits which may be separated from the underlying regional aquifer by a low permeability or confining layer. This confining layer typically “leaks”, providing recharge to the deeper zones.

11) Coastal Beaches

This hydrogeologic environment is characterized by low topographic relief, near sea-level elevation and unconsolidated deposits of water-washed sands. The term beach is appropriately applied only to a body of essentially loose sediment. This usually means sand-size particles, but could include gravel. Quartz particles usually predominate. These materials are well sorted, very permeable and have very high potential infiltration rates. These areas are commonly ground-water discharge areas although they can be very susceptible to the intrusion of saltwater.

12) Solution Limestone

Large portions of the central and southeastern United States are underlain by limestones and dolomites in which the fractures have been enlarged by solution. Although ground water occurs in both the surficial deposits and in the underlying bedrock, the limestones and dolomites, which typically contain solution cavities, generally serve as the principal aquifers. This type of hydrogeologic environment is often described as “karst.”

13) Unknown Environment

If the subsurface hydrogeological environment is unknown, or it is different from any of the twelve main types used in EPACMTP, select the subsurface environment as Type 13. In this case, EPACMTP will assign values of the hydrogeological parameters (depth to ground water, saturated zone thickness, saturated zone hydraulic conductivity, and saturated zone hydraulic gradient) that are simply national average values.

Data Sources

In the absence of site-specific data, default distributions of values can be used for the following aquifer characteristics: depth to ground water and aquifer thickness, hydraulic conductivity, and hydraulic gradient. These default distributions are derived from the Hydrogeologic Database for Ground-Water Modeling (HGDB), assembled by Rice University on behalf of the American Petroleum Institute (API) (Newell et al., 1990) and are linked to the WMU sites in the site data file using the hydrogeologic environment index.

Use In EPACMTP

EPACMTP includes a database of aquifer characteristics for 13 hydrogeologic environments. The hydrogeologic environment index is a sequential number assigned to each hydrogeologic environment in the default database included with EPACMTP in order to provide a simple means of specifying which correlated set of aquifer characteristics should be used to model the given WMU site using the regional site-based modeling methodology.

5.3.4.3 Saturated Zone Thickness (B)

Definition

The saturated zone thickness is the vertical thickness of the zone in which the voids in the rock or soil are filled with water at a pressure greater than atmospheric. In an unconfined aquifer such as that simulated by the EPACMTP model, the water table is at the top of the saturated zone. Usually the base of the saturated zone is an impermeable layer, e.g., bedrock.

Parameter Value or Distribution of Values

If site-specific data are available, then the saturated zone thickness can be specified in the input file as a constant value or an empirical or statistical distribution of values. In this case, if your site has a highly stratified hydrogeology, it may be difficult to precisely define the “base of the aquifer,” but the stratification may effectively limit the vertical plume travel distance, so it may be appropriate to enter the maximum vertical extent of the plume as an “effective” saturated zone thickness.

Lacking site-specific data, a default distribution of saturated zone thickness values may be used as part of the regional site-based modeling methodology. As described in Section 5.5 of the *EPACMTP Technical Background Document* (U.S. EPA, 2003a), the regional site-based modeling methodology is an attempt to ensure that the combination of parameter values that is randomly generated by the Monte Carlo module of EPACMTP represents a realistic set of site conditions. The cumulative frequency distribution of saturated zone thickness listed in Table 5.20 was generated by performing a default landfill modeling analysis using the regional site-based modeling methodology; the entire Hydrogeologic Database for Modeling (HGDB) from which these values were derived is presented in Appendix D. For a

given percentile (%) frequency and value pair in Table 5.20, the percentile denotes the relative frequency or likelihood of parameter values in the entire distribution being less than or equal to the corresponding parameter value in the right hand column.

Table 5.20 Cumulative Frequency Distribution of Saturated Zone Thickness

%	Saturated Zone Thickness (m)
0	3.05E-01
10	4.27E+00
25	7.62E+00
50	1.43E+01
75	3.24E+01
80	4.83E+01
85	6.66E+01
90	9.14E+01
95	1.52E+02
100	9.14E+02

Data Sources

In the regional site-based Monte Carlo analysis used for nationwide modeling applications, the distribution of values for the thickness of the saturated zone is produced through Monte Carlo sampling of the HGDB, based on the hydrogeologic environment assigned to the waste site selected (from the default database) for each model realization. The HGDB (Newell et al., 1990; U.S. EPA, 1997d) is an empirical database of aquifer characteristics developed from a survey of hazardous waste sites in the United States that provides data on hydrogeologic parameters (aquifer thickness, unsaturated zone thickness, hydraulic gradient and hydraulic conductivity) that are required by the EPACMTP model. The HGDB from which the values shown in Table 5.20 were derived is presented in its entirety in Appendix D.

In a location-specific modeling analysis, saturated zone thickness must be derived from a site-specific data source and specified in the input file as a constant value or an empirical or statistical distribution of values.

Use In EPACMTP

The thickness of the saturated zone is an input to the saturated zone flow module. It is used in EPACMTP to describe the thickness of the ground-water zone over which the leachate plume can mix with ground water and impacts the dilution rates in the saturated zone.

5.3.4.4 Hydraulic Conductivity (K)

Definition

Hydraulic conductivity is a measure of the ability to transmit water under a unit hydraulic gradient.

Parameter Value or Distribution of Values

If site-specific data are available, then the hydraulic conductivity can be specified in the input file as a constant value or an empirical or statistical distribution of values.

Lacking site-specific data, a default distribution of hydraulic conductivity values may be used as part of the regional site-based modeling methodology. As described in Section 5.5 of the *EPACMTP Technical Background Document* (U.S. EPA, 2003a), the regional site-based modeling methodology is an attempt to ensure that the combination of parameter values that is randomly generated by the Monte Carlo module of EPACMTP represents a realistic set of site conditions. The cumulative frequency distribution of hydraulic conductivity listed in Table 5.21 was generated by performing a default nationwide landfill modeling analysis using the regional site-based modeling methodology; the entire Hydrogeologic Database for Modeling (HGDB) from which these values were derived is presented in Appendix D. For a given percentile (%) frequency and value pair in Table 5.21, the percentile denotes the relative frequency or likelihood of parameter values in the entire distribution being less than or equal to the corresponding parameter value in the right hand column.

Table 5.21 Cumulative Frequency Distribution of Hydraulic Conductivity

%	Hydraulic Conductivity (m/yr)
0	3.15E+00
10	1.73E+02
25	8.04E+02
50	1.89E+03
75	1.10E+04
80	1.39E+04
85	2.21E+04
90	3.15E+04
95	7.48E+04
100	4.29E+06

Alternatively, the hydraulic conductivity can be specified as a derived parameter. In this case it is calculated within EPACMTP from the particle diameter using the Kozeny-Carman equation (Bear, 1979) shown below:

$$K = \frac{\rho g}{\mu} \frac{\phi^2}{(1-\phi)} \frac{d^2}{1.8} \quad (5.7)$$

where:

- K = hydraulic conductivity (cm/s)
- ρ = density of water (kg/m³)
- g = acceleration due to gravity (m/s²)
- μ = dynamic viscosity of water (N-s/m²)
- d = mean particle diameter (m)
- ϕ = total porosity of the aquifer material (dimensionless)

In Equation 5.7 shown above, the constant 1.8 includes a unit conversion factor to yield K in units of cm/s. Both the density and the dynamic viscosity of water are functions of temperature and are computed using the regression equations presented in CRC (1981).

Data Sources

In the regional site-based Monte Carlo analysis used for nationwide modeling applications, the distribution of values for the hydraulic conductivity is produced through Monte Carlo sampling of the HGDB, based on the hydrogeologic environment assigned to the waste site selected (from the default database) for each model realization. The HGDB (Newell et al., 1990; U.S. EPA, 1997d) is an empirical database of aquifer characteristics developed from a survey of hazardous waste sites in the United States that provides data on hydrogeologic parameters (aquifer thickness, unsaturated zone thickness, hydraulic gradient and hydraulic conductivity) that are required by the EPACMTP model. The HGDB from which the values shown in Table 5.21 were derived is presented in its entirety in Appendix D.

If specified as a derived parameter, the aquifer hydraulic conductivity is calculated from the mean particle diameter using the Kozeny-Carman equation (Bear, 1979).

In a location-specific modeling analysis, hydraulic conductivity must be derived from a site-specific data source and specified in the input file as a constant value or an empirical or statistical distribution of values.

Use In EPACMTP

The aquifer hydraulic conductivity is an input to the saturated zone flow module. The hydraulic conductivity, together with the hydraulic gradient, controls the ground-water flow rate. Assigning a low hydraulic conductivity value will not necessarily result in lower predicted ground-water exposures. In a broader sense, it means that siting a WMU in a low permeability aquifer setting is not always more protective than a high permeability setting. Low ground-water velocity means that it

will take longer for the exposure to occur, and as a result, there is more opportunity for natural attenuation to degrade contaminants. However, for long-lived waste constituents, it also means that little dilution of the plume may occur.

5.3.4.5 Regional Hydraulic Gradient (r)

Definition

Hydraulic gradient measures the head difference between two points as a function of their distance. For an unconfined aquifer such as that modeled with EPACMTP, the hydraulic gradient is simply the slope of the water table in a particular direction. It is calculated as the difference in the elevation of the water table measured at two locations divided by the distance between the two locations. In EPACMTP, this parameter represents the average horizontal ground-water gradient in the vicinity of the WMU location. The gradient is meant to represent the 'natural' ground-water gradient as it is, or would be, without influence from the WMU. The presence of a WMU, particularly a surface impoundment, may cause local mounding of the water table and associated higher local ground-water gradients. The EPACMTP model assumes that the gradient value specified in the input file does not include mounding; rather, the model will calculate the predicted impact on the ground water of the WMU and liner design (if any) as part of the modeling evaluation.

Parameter Value or Distribution of Values

If site-specific data are available, then the regional hydraulic gradient can be specified in the input file as a constant value or an empirical or statistical distribution of values.

Lacking site-specific data, a default distribution of regional hydraulic gradient values may be used as part of the regional site-based modeling methodology. As described in Section 5.5 of the *EPACMTP Technical Background Document* (U.S. EPA, 2003a), the regional site-based modeling methodology is an attempt to ensure that the combination of parameter values that is randomly generated by the Monte Carlo module of EPACMTP represents a realistic set of site conditions. The cumulative frequency distribution of regional hydraulic gradient listed in Table 5.22 was generated by performing a default nationwide landfill modeling analysis using the regional site-based modeling methodology; the entire Hydrogeologic Database for Modeling (HGDB) from which these values were derived is presented in Appendix D. For a given percentile (%) frequency and value pair in Table 5.22, the percentile denotes the relative frequency or likelihood of parameter values in the entire distribution being less than or equal to the corresponding parameter value in the right hand column.

Table 5.22 Cumulative Frequency Distribution of Regional hydraulic gradient

%	Regional Hydraulic Gradient (unitless)
0	2.00E-06
10	9.00E-04
25	2.00E-03
50	5.70E-03
75	1.51E-02
80	2.00E-02
85	2.46E-02
90	3.10E-02
95	4.90E-02
100	4.91E-01

Data Sources

In the regional site-based Monte Carlo analysis used for nationwide modeling applications, the distribution of values for the regional hydraulic gradient is produced through Monte Carlo sampling of the HGDB, based on the hydrogeologic environment assigned to the waste site selected (from the default database) for each model realization. The HGDB (Newell et al., 1990; U.S. EPA, 1997d) is an empirical database of aquifer characteristics developed from a survey of hazardous waste sites in the United States that provides data on hydrogeologic parameters (aquifer thickness, unsaturated zone thickness, hydraulic gradient and hydraulic conductivity) that are required by the EPACMTP model. The HGDB from which the values shown in Table 5.22 were derived is presented in its entirety in Appendix D.

In a location-specific modeling analysis, regional hydraulic gradient must be derived from a site-specific data source and specified in the input file as a constant value or an empirical or statistical distribution of values.

Use In EPACMTP

The hydraulic gradient and the hydraulic conductivity (see Section 5.3.4.4) are inputs to the saturated zone flow module, and together they control the ground-water flow rate, in accordance with Darcy's Law. The effect of varying ground-water flow rate on contaminant fate and transport is complex. Intuitively, it would seem that factors that increase the ground-water flow rate would cause a higher ground-water exposure level at the receptor well, but this is not always the case. A higher ground-water velocity will cause leachate constituents to arrive at the well location more quickly. For constituents that are subject to degradation in ground water, the shorter travel time will cause the constituents to arrive at the well at higher concentrations as compared to a case of low ground-water velocity and long travel times. On the other hand, a high ground-water flow rate will tend to increase the degree of dilution of the leachate plume, due to mixing and dispersion. This will in turn tend to lower the magnitude of the concentrations reaching the well. The

modeling scenario evaluated in EPACMTP is based on the maximum constituent concentrations at the well (either a peak concentration or the maximum time-averaged concentration), rather than how long it might take for that exposure to occur. Therefore, a higher ground-water flow rate may result in lower predicted exposure levels at the well.

5.3.5 Seepage Velocity (V_x)

Definition

Seepage velocity is the average linear velocity of a water particle in a ground water system. It is equal to the Darcy velocity divided by effective porosity.

Parameter Value or Distribution of Values

The ground-water seepage velocity is related to the aquifer properties through Darcy's law. The regional seepage velocity may be input directly, as a constant value or a distribution of values. If site specific data are not available, it may be specified in the input file as a derived parameter. In this case, it is computed as:

$$V_x = \frac{K_x}{\phi_e} r \quad (5.8)$$

where

- V_x = longitudinal ground water seepage velocity (in the x-direction) (m/yr)
- K_x = longitudinal hydraulic conductivity (in the x-direction) (m/yr)
- r = regional hydraulic gradient (dimensionless)
- ϕ_e = effective porosity (dimensionless)

Default lower and upper bounds for the seepage velocity are 0.1 and 1.1×10^4 m/yr, respectively. This range of values is based on survey data reported by Newell et al (1990).

The cumulative frequency distribution for the seepage velocity listed in Table 5.23 was generated by performing a default nationwide landfill modeling analysis using the regional site-based modeling methodology. For a given percentile (%) frequency and value pair in this table, the percentile denotes the relative frequency or likelihood of parameter values in the entire distribution being less than or equal to the corresponding parameter value in the right hand column.

Table 5.23 Cumulative Frequency Distribution of Ground-water Seepage Velocity

%	Seepage Velocity (m/yr)
0	2.17E+00
10	5.99E+00
25	5.11E+00
50	4.08E+01
75	6.73E+02
80	4.02E+02
85	2.53E+00
90	6.57E+00
95	2.27E+00
100	4.13E+01

Data Sources

In the regional site-based Monte Carlo analysis that is typically used for nationwide modeling applications, the seepage velocity is, by default, internally derived using the correlated values for hydraulic conductivity and gradient that are produced through Monte Carlo sampling of the HGDB, based on the hydrogeologic environment assigned to the waste site selected for each model realization. The default lower and upper bounds for this input are based on survey data reported by Newell et al (1990).

If specified as a derived parameter, the regional ground-water seepage velocity is calculated from the hydraulic conductivity and gradient, and the aquifer porosity using Equation 5.8 with upper and lower bounds based on survey data reported by Newell et al (1990).

In a location-adjusted or quasi-site-specific modeling analysis, the site-specific hydraulic gradient must be derived from a site-specific data source and specified in the input file as a constant value or an empirical or statistical distribution of values.

Use In EPACMTP

The seepage velocity that is provided as an EPACMTP input parameter represents ambient ground water flow conditions, that is, without the WMU present. The EPACMTP saturated zone flow module calculates the final distribution of seepage velocities in the model domain, taking into account infiltration from the WMU. These calculated seepage velocities are then used in the saturated zone transport module to simulate the fate and transport of leachate constituents.

5.3.6 **Anisotropy Ratio (A_r)**

Definition

The anisotropy ratio is a factor used to specify the relationship between the horizontal and vertical aquifer hydraulic conductivities. It is defined as the ratio of the horizontal hydraulic conductivity to the vertical hydraulic conductivity.

Parameter Value or Distribution of Values

Although the aquifer properties are assumed to be uniform, the EPACMTP model can accommodate the situation where the horizontal and vertical aquifer hydraulic conductivities are different. The anisotropy ratio is a factor used to specify the relationship between these two hydraulic conductivity values and is defined according to the following equation:

$$A_r = K_x / K_z \quad (5.9)$$

where:

$$\begin{aligned} A_r &= \text{anisotropy ratio} = K_x / K_z \\ K_x &= \text{hydraulic conductivity in the x direction (m/yr)} \\ K_z &= \text{hydraulic conductivity in the z direction (m/yr)} \end{aligned}$$

The default value of A_r is 1, which indicates an isotropic system. Note that in the EPACMTP model, the horizontal transverse hydraulic conductivity is assumed to be equal to the horizontal longitudinal conductivity, i.e., $K_y = K_x$.

Data Sources

Because anisotropy ratios observed in the field may commonly be on the order of 100:1 or even larger (Freeze and Cherry, 1979), a uniform distribution of A_r with limits of 1 and 100 may be reasonable for some applications of the model. However, for nationwide assessment purposes, the default value of A_r is 1, which indicates an isotropic system.

Use In EPACMTP

The anisotropy ratio is used to estimate the vertical conductivity from the horizontal conductivity. However, by default, the vertical conductivity is set equal to the horizontal conductivity. The horizontal and vertical conductivities are inputs to the saturated zone flow module.

5.3.7 Retardation Coefficient for the Saturated Zone (R^s)

Definition

The retardation coefficient is a measure of the degree to which contaminant velocities are retarded relative to that of the bulk mass of ground water within the aquifer. A value of 1.0 indicates that the constituent is conservative; in other words, it is not subject to adsorption and travels at the same speed as the bulk mass of ground-water. Values greater than 1.0 indicate that the constituent transport is retarded due to adsorption.

Parameter Value or Distribution of Values

In most modeling applications using EPACMTP, the retardation coefficient is specified as a derived variable; however, if site-specific data are available, this input parameter can be set to a constant value or a distribution of values.

For constituents modeled with a linear adsorption isotherm (typically, organics and metals modeled with a pH-dependent isotherm or a constant k_d value), when the retardation coefficient is specified as a derived variable in the EPACMTP input file, it is calculated according to the following equation:

$$R^s = 1 + \frac{\rho_b K_d}{\phi} \quad (5.10)$$

where

R^s = retardation coefficient for the saturated zone (dimensionless)

ρ_b = bulk density of the porous media [g/cm³]

k_d = distribution coefficient [cm³/g]

ϕ = porosity

For constituents modeled with a nonlinear adsorption isotherm (that is, R^s is no longer constant but is a function of metal concentration), R^s must be specified in the input file as a derived variable and the K_d -concentration relation must be specified by the user in one of two ways: 1) in terms of the two Freundlich parameters (k_f and n_f ; see Sections 5.3.12 and 5.3.13); or 2) in terms of the tabulated MINTEQA2-derived isotherms (see Section 3.3.3.2).

For the modeling of metals, the EPACMTP user has three options for specifying the relationship between dissolved and adsorbed concentrations: 1) MINTEQA2-derived non-linear isotherms, 2) pH-dependent empirical isotherms, or 3) an empirical distribution of values. In the case of the first option, the non-linear isotherm is only used in the unsaturated zone; a linear sorption isotherm (e.g., an effective K_d value) is used for the saturated zone. This effective K_d value is determined from the maximum contaminant concentration at the water table and

values of the five environmental master variables (pH, iron-oxide, leachate organic matter, natural organic matter in the aquifer, and ground water environment type (carbonate or non-carbonate)), following the procedure described in Appendix B.

Data Sources

Lacking site-specific data, Equation 5.10 is used to calculate the retardation coefficient for constituents that are modeled using a linear adsorption isotherm. For constituents modeled with a non-linear adsorption isotherm, the effective retardation coefficient is calculated inside EPACMTP, based upon the nonlinear concentration- K_d relationship as given by MINTEQA2-derived isotherms.

Use In EPACMTP

The retardation coefficient is an input to the saturated zone transport module.

5.3.8 Dispersivity

The transport of the contaminant plume in the saturated zone is controlled by two mechanisms: advection and dispersion. The EPACMTP saturated zone flow module simulates both of these mechanisms. Dispersion is the phenomenon by which a constituent plume in flowing ground water is mixed with uncontaminated water and becomes reduced in concentration at the perimeter of the plume. Not all of a contaminant plume is traveling at the same velocity due to differences in pore size and flow path length and friction along pore walls, resulting in mixing along the flow path which decreases solute concentrations. Note that the saturated zone dispersivity is measured in three directions: longitudinal (along the flow path, or in the x-direction), horizontal transverse (perpendicular to the flow path, or in the y-direction), and vertical (in the z-direction).

The model computes the longitudinal, horizontal transverse, and vertical dispersion coefficients as the product of the seepage velocity and longitudinal (α_L), transverse (α_T) and vertical (α_V) dispersivities. A literature review indicated the absence of a generally accepted theory to describe dispersivities, although a strong dependence on scale has been noted (EPRI, 1985; Gelhar, Welty, and Rehfeldt, 1992). In the absence of user-specified values or distributions, the longitudinal dispersivity is represented through a probabilistic formulation and the horizontal transverse and vertical dispersivities are, by default, calculated from the longitudinal dispersivity, as described below.

For non-degrading contaminants, the dilution caused by dispersive mixing is a controlling factor in determining the concentration observed at a receptor well. However, in Monte Carlo analyses involving varying well location, the predicted maximum well concentration is relatively insensitive to dispersion. The reason for this is as follows: low dispersivities will lead to a compact, concentrated plume. If the plume is relatively small, the likelihood that the receptor well will intercept the plume is reduced, but the concentration in the well, if it does, will be high. High dispersivities will lead to a more dilute plume which occupies a greater volume,

thereby increasing the likelihood that a receptor well will intercept the plume. Concentrations in the plume, however, are likely to be lower than in the first case. In the course of a full Monte Carlo analysis, these effects will tend to compensate for each other.

5.3.8.1 Longitudinal Dispersivity (α_L)

Definition

Dispersion is the phenomenon by which a contaminant plume in flowing ground water is mixed with uncontaminated water and becomes reduced in concentration at the perimeter of the plume. The longitudinal dispersivity is the characteristic length that defines spatial extent of dispersion of contaminants, measured in the longitudinal direction, that is, along the flow path or in the x-direction.

Parameter Value or Distribution of Values

If site-specific data are available, then the longitudinal dispersivity can be specified in the input file as a constant value or an empirical or statistical distribution of values.

In the absence of site-specific data, the longitudinal dispersivity is, by default, represented through a probabilistic formulation as shown in Table 5.24, and the horizontal transverse and vertical dispersivities are then calculated from the longitudinal dispersivity. The distribution shown in Table 5.24 is based on data presented in EPRI (1985). For a given percentile (%) frequency and value pair in this table, the percentile denotes the relative frequency or likelihood of parameter values in the entire distribution being less than or equal to the corresponding parameter value in the right hand column. Within each of the three classes shown in Table 5.24, the longitudinal dispersivity is assumed to be uniform. Note that the values of longitudinal dispersivity in this table are based on a receptor well distance of 152.4 m. For distances other than 152.4 m, the following equations are used:

$$\alpha_L(x_t) = \alpha_{Ref}(x_t = 152.4) (x_t / 152.4)^{0.5} \quad (5.11)$$

where: $x_t = 0.5 x_w + x_r \quad (5.12)$

α_L	=	longitudinal dispersivity (m)
x_t	=	average travel distance in the x direction (m)
x_w	=	length of the WMU in the x-direction (parallel to ground water flow) (m)
x_{rw}	=	distance from the downgradient boundary of the WMU to the receptor well (m)
α_{Ref}	=	reference longitudinal dispersivity, as determined from the probabilistic distribution (m)

Table 5.24 Probabilistic representation of longitudinal dispersivity

%	α_L (m)*
0	0.1
10	1.0
70	10.0
100	100.0

*Assumes $x_t = 152.4$ m (see Equation 5.11)

In other words, the travel distance x_t is equal to the distance between the receptor well and the downgradient facility boundary (x_{rw}), plus one-half of the facility dimension. The average distance for all of the contaminants to migrate to the edge of the waste management unit is equal to one half the length of the unit or $\frac{1}{2} x_w$. The default minimum value of α_L is 0.1 m.

Table 5.25 lists the cumulative frequency distribution of longitudinal dispersivity that is generated in a default landfill modeling analysis using the regional site-based modeling methodology. For a given percentile (%) frequency and value pair in this table, the percentile denotes the relative frequency or likelihood of parameter values in the entire distribution being less than or equal to the corresponding parameter value in the right hand column.

Table 5.25 Cumulative Frequency Distribution of Longitudinal Dispersivity

%	Longitudinal Dispersivity (m)
0	1.00E-01
10	1.22E+00
25	3.62E+00
50	8.96E+00
75	2.54E+01
80	4.32E+01
85	6.53E+01
90	9.21E+01
95	1.35E+02
100	3.18E+02

Data Sources

The relationship in Equation 5.11 was derived based on a professional review of data presented in EPRI (1985). More recently, Gelhar et al. (1992) have compiled and documented results from a large number of studies in which dispersivity values have been reported. These studies represent a wide range of spatial scales, from a few meters to more than 10,000 meters. The data as presented by Gelhar et al. (1992) show a clear correlation between scale and apparent dispersivity. Equation 5.11 used in EPACMTP describes the observed data reasonably well. The field data suggest a somewhat steeper slope of the distance-dispersivity relation on a log-log scale than is used in the modeling analyses. However, a sensitivity analysis performed using EPACMTP (HydroGeoLogic, 1992) has shown that the model results are virtually identical when the slope is varied from 0.5 to 1.5. For this reason the original relationship as shown in Equation 5.11 has been retained.

The data presented by Gelhar et al. (1992) also show that the ratios between longitudinal, and horizontal and vertical transverse dispersivities used in the nationwide modeling, are consistent with published data.

Use In EPACMTP

The longitudinal dispersivity is an input to the saturated zone transport module.

5.3.8.2 Horizontal Transverse Dispersivity (α_T)

Definition

Dispersion is the phenomenon by which a contaminant plume in flowing ground water is mixed with uncontaminated water and becomes reduced in concentration at the perimeter of the plume. The horizontal transverse dispersivity is the characteristic length that defines spatial extent of dispersion of contaminants, measured in the horizontal transverse direction, that is, perpendicular to the flow path, or in the y-direction.

Parameter Value or Distribution of Values

If site-specific data are available, then the horizontal transverse dispersivity can be specified in the input file as a constant value or an empirical or statistical distribution of values.

In the absence of site-specific data, the horizontal transverse dispersivity is, by default, calculated from the longitudinal dispersivity using the following equation:

$$\alpha_T = \alpha_L / 8 \quad (5.13)$$

where:

α_L = longitudinal dispersivity (m)
 α_T = horizontal transverse dispersivity (m)

Note that in EPACMTP, the input value for α_T is actually the ratio of α_L to α_T . Although the user can define a different value for the ratio of the longitudinal to the transverse dispersivity, the ratio of $\alpha_L/\alpha_T = 8$ is used by default.

Table 5.26 lists the cumulative frequency distribution of horizontal transverse dispersivity that is generated in a default landfill modeling analysis using the regional site-based modeling methodology. For a given percentile (%) frequency and value pair in this table, the percentile denotes the relative frequency or likelihood of parameter values in the entire distribution being less than or equal to the corresponding parameter value in the right hand column.

Table 5.26 Cumulative Frequency Distribution of Horizontal Transverse Dispersivity

%	Horizontal Transverse Dispersivity (m)
0	1.25E-02
10	1.53E-01
25	4.52E-01
50	1.12E+00
75	3.17E+00
80	5.40E+00
85	8.16E+00
90	1.15E+01
95	1.69E+01
100	3.97E+01

Data Sources

By default, the transverse (α_T) dispersivity is calculated by the EPACMTP model as a fraction of the longitudinal dispersivity. The dispersivity relationship described above has been derived based on a professional review of data presented in EPRI (1985). More recently, Gelhar et al. (1992) have compiled and documented results from a large number of studies in which dispersivity values have been reported. The data presented by Gelhar et al. (1992) show that this default ratio between longitudinal and horizontal transverse dispersivities is consistent with published data.

Use In EPACMTP

The horizontal transverse dispersivity is an input to the saturated zone transport module.

5.3.8.3 Vertical Dispersivity (α_v)
Definition

Dispersion is the phenomenon by which a contaminant plume in flowing ground water is mixed with uncontaminated water and becomes reduced in concentration at the perimeter of the plume. The vertical dispersivity is the characteristic length that defines spatial extent of dispersion of contaminants, measured vertically downward or in the z-direction.

Parameter Value or Distribution of Values

If site-specific data are available, then the vertical dispersivity can be specified in the input file as a constant value or an empirical or statistical distribution of values.

In the absence of site-specific data, the vertical dispersivity is, by default, calculated from the longitudinal dispersivity using the following equation:

$$\alpha_v = \alpha_L / 160 \quad (5.14)$$

where:

$$\begin{array}{ll} \alpha_L & = \text{longitudinal dispersivity (m)} \\ \alpha_v & = \text{vertical dispersivity (m)} \end{array}$$

Note that in EPACMTP, the input value for α_v is actually the ratio of α_L to α_v . Although the user can define a different value for the ratio of the longitudinal to the vertical dispersivity, the ratio of $\alpha_L/\alpha_v = 160$ is used by default.

Table 5.27 lists the cumulative frequency distribution of horizontal transverse dispersivity that is generated in a default landfill modeling analysis using the regional site-based modeling methodology. For a given percentile (%) frequency and value pair in this table, the percentile denotes the relative frequency or likelihood of parameter values in the entire distribution being less than or equal to the corresponding parameter value in the right hand column.

Table 5.27 Cumulative Frequency Distribution of Vertical Dispersivity

%	Vertical Dispersivity (m)
0	1.00E-02
10	1.00E-02
25	2.26E-02
50	5.60E-02
75	1.58E-01
80	2.70E-01
85	4.08E-01
90	5.76E-01
95	8.45E-01
100	1.99E+00

Data Sources

By default, the vertical (α_v) dispersivity is calculated by the EPACMTP model as a fraction of the longitudinal dispersivity. The dispersivity relationship described above has been derived based on a review of available data. More recently, Gelhar et al. (1992) have compiled and documented results from a large number of studies in which dispersivity values have been reported. The data presented by Gelhar et al. (1992) show that this default ratio between longitudinal and vertical dispersivities is consistent with published data.

Use In EPACMTP

The vertical dispersivity is an input to the saturated zone transport module; dispersion in the saturated zone generally tends to decrease contaminant concentrations at the receptor well.

5.3.9 Aquifer Temperature (T)**Definition**

The aquifer temperature is the long-term average temperature of the ground water within the aquifer. Note that although the temperature of the ground water within the vadose zone is not an explicit model input, this temperature is assumed by EPACMTP to be the same as that of the aquifer.

Parameter Value or Distribution of Values

As modeled in EPACMTP, aquifer temperature affects the transformation rate of constituents that are subject to hydrolysis, through the effect of temperature on reaction rates (see Section 3.3.2.2). In the development of the site data files for each WMU type, information on average annual temperatures in shallow ground-water systems (Todd, 1980) to assign a temperature value to each WMU in the

modeling database, based on the unit's geographical location. For each WMU site, the assigned temperature was an average of the upper and lower values for that temperature region, as shown in Figure 5.3. In other words, all WMU's located in the band between 10° and 15° were assigned a temperature value of 12.5 °C.

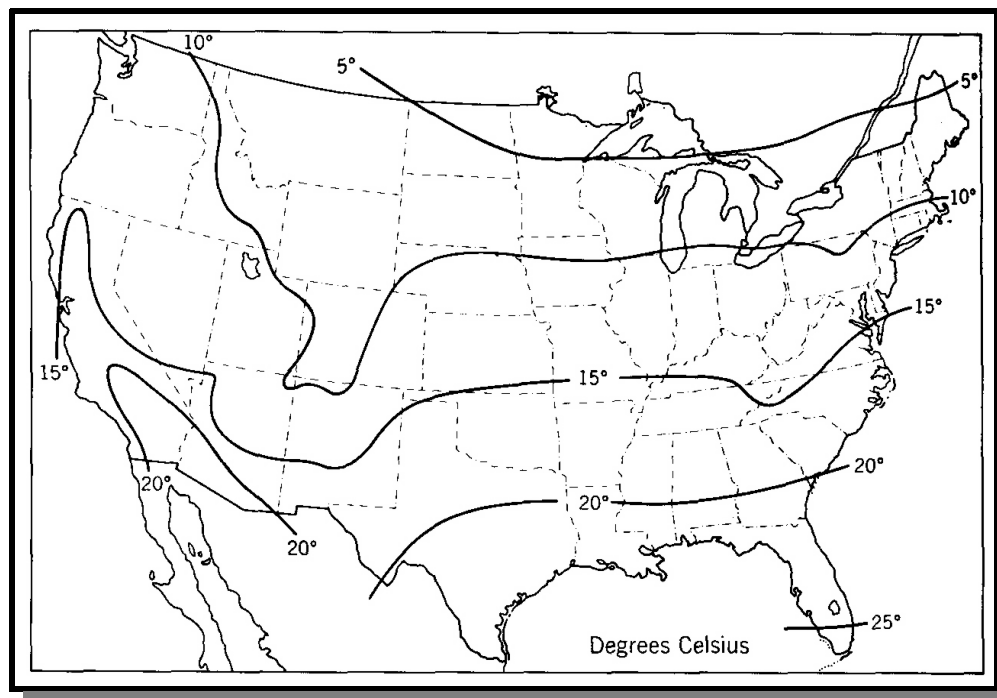


Figure 5.3 Ground-water Temperature Distribution for Shallow Aquifers in the United States (from Todd, 1980)

Data Sources

We used information on average annual temperatures in shallow ground-water systems from Todd (1980) to assign a temperature value to each WMU site in the site data files, based on the unit's geographical location.

Use In EPACMTP

When the EPACMTP model is run using the regional, site-based methodology, the model selects a site at random from those in the site data file for each Monte Carlo realization. For each WMU site, the ground-water temperature was assigned using the data from Todd, (1980) and the unit's geographical location.

In a location-adjusted modeling analysis, a site-specific ground-water temperature can be directly specified in the input file – either as constant value or as a statistical or empirical distribution of values.

The aquifer temperature associated with the modeled site and the specified hydrolysis rate constants are then used by the model to derive the appropriate temperature-dependent first-order hydrolysis rate for organic constituents. Note that although the temperature of the ground water within the vadose zone is not an explicit model input, the EPACMTP model assumes that the soil temperature is the same as that of the aquifer.

5.3.10 Ground-water pH (pH)

Definition

A measure of the acidity or alkalinity of the ground water, pH is measured on a scale of 0 to 14, with 7 representing a neutral state. Values less than 7 are acidic, and values greater than 7 are basic. pH is calculated as the negative logarithm of the concentration of hydrogen ions in a solution. For modeling purposes, the EPACMTP model assumes subsurface pH value is the same in the unsaturated zone and saturated zone.

Parameter Value or Distribution of Values

If site-specific data are available, then the ground-water pH can be specified in the input file as a constant value or an empirical or statistical distribution of values.

Lacking site-specific data, a default distribution of pH values may be used. This pH distribution was obtained through analysis of nearly 25,000 field-measured pH values of uncontaminated ground water obtained from EPA's STORET database (U.S. EPA, 1996). The data are represented by an empirical distribution with low and high values of 3.2 and 9.7, respectively and a median value of 6.8. Because the STORET database has unrealistic extreme values (presumably from errors in instrument calibration or reading, or in data entry), the upper and lower bounds of the distribution were established by reference to reported values in the open literature. The resulting pH distribution is shown in Table 5.28. For a given percentile (%) frequency and value pair in this table, the percentile denotes the relative frequency or likelihood of parameter values in the entire distribution being less than or equal to the corresponding parameter value in the right hand column.

Table 5.28 Probability distribution of aquifer pH

%	Ground-water pH (standard units)
0	4.32E+00
10	7.49E+00
25	7.30E+00
50	8.91E+00
75	7.84E+00
80	7.43E+00
85	4.65E+00
90	7.42E+00
95	5.74E+00
100	4.87E+00

Note that these values generated for the ground-water pH is assumed to apply to the unsaturated zone as well. The EPACMTP model assumes that the ground-water/aquifer system is well buffered with respect to pH. That is, in the modeling analysis, there is no effect on the ambient pH from the leachate emanating from the base of the WMU. Additionally, the generated pH value is assumed to apply to both the unsaturated zone and saturated zone.

Data Sources

The distribution of pH values shown in Table 5.28 was obtained through analysis of nearly 25,000 field measured pH values of uncontaminated ground water obtained from EPA's STORET database (U.S. EPA, 1996). Note that the upper and lower bounds of this distribution were established by reference to reported values in the open literature.

Use In EPACMTP

The ground-water pH is one of the most important subsurface parameters controlling the mobility of metals. Most metals are more mobile under acidic (low pH) conditions, as compared to neutral or alkaline (pH of 7 or higher) conditions. The pH may also affect the hydrolysis rate of organic constituents; some constituents degrade more rapidly or more slowly as pH varies. The pH of most aquifer systems is slightly acidic, the primary exception being aquifers in solution limestone settings. These may also be referred to as 'karst', 'carbonate' or 'dolomite' aquifers. The ground water in these systems is usually alkaline.

5.3.11 Fractional Organic Carbon Content (f_{oc}^s)

Definition

The nature and amount of solid matter in the subsurface to which chemical constituents are attracted (the adsorbent) are important in determining the extent to which a constituent's transport through the ground-water pathway is retarded due to adsorption. Particulate organic matter present in the saturated zone (input to EPACMTP as fraction organic carbon) represents one of the dominant adsorbents for sorption of both organic and metal constituents in environmental systems and was one of the geochemical master variables used in the calculation of the non-linear sorption isotherms using the MINTEQA2 model.

Parameter Value or Distribution of Values

If site-specific data are available, then the fractional organic carbon content of the aquifer can be specified in the input file as a constant value or an empirical or statistical distribution of values.

Lacking site-specific data, a default distribution of values may be used. Unfortunately, few if any comprehensive subsurface characterizations of organic carbon content exist. In general, the reported values are low, typically less than 0.01. For the purposes of modeling organic constituents, a low range of values was assumed and the distribution shape was based on the distribution of measured dissolved organic carbon recorded in EPA's STORET data base. The default distribution for fractional organic carbon content is a Johnson SB distribution with a mean and standard deviation in arithmetic space of 4.32×10^{-4} and 0.0456, respectively and upper and lower limits of 0.064 and 0.0, respectively. In the case of metals, the sorption is controlled by complex geochemical interactions which are simulated using MINTEQA2 (see Section 3.3.3.2 and Appendix B), and this distribution of f_{oc} is not used.

A summary of this default distribution is presented in Table 5.29. For a given percentile (%) frequency and value pair in this table, the percentile denotes the relative frequency or likelihood of parameter values in the entire distribution being less than or equal to the corresponding parameter value in the right hand column.

Table 5.29 Probability distribution of fraction organic carbon in the saturated zone

%	Fractional Organic Carbon Content (unitless)
0	6.77E-04
10	4.11E-03
25	8.51E-04
50	1.10E-04
75	4.71E-04
80	7.82E-04
85	3.01E-04
90	9.99E-04
95	5.99E-04
100	7.93E-04

Data Sources

The default distribution for f_{oc} was derived based on professional judgement and the distribution shape was based on the distribution of measured dissolved organic carbon recorded in EPA's STORET database.

Use In EPACMTP

The organic carbon content, f_{oc} , is used to determine the linear distribution coefficient, K_d . This approach is valid only for organic contaminants containing hydrophobic groups since these constituents tend to sorb preferentially on non-polar natural organic compounds in the soil or aquifer. In the case of metals, the organic matter content in the subsurface is one of the controlling master variables used to develop the MINTEQA2-derived isotherms, and EPACMTP uses this organic matter content to select appropriate isotherms to use during the EPACMTP simulation process.

5.3.12 Leading Coefficient of Freundlich Isotherm for Saturated Zone (K_d^s)**Definition**

The leading coefficient of the Freundlich isotherm is a constant used to describe the sorptive behavior of a constituent. When the sorption data are plotted as $\log C$ versus $\log S$, the intercept of the resulting line is equal to $\log K^s$. In the special case of a linear isotherm, the leading Freundlich coefficient is known as the linear solid-liquid phase distribution coefficient (K_d^s) (commonly called the distribution coefficient).

Parameter Value or Distribution of Values

When modeling organic constituents with EPACMTP, the leading Freundlich coefficient is generally specified as a derived parameter in the input file. If derived, the leading Freundlich coefficient (K_d^s) is automatically assumed linear and calculated by the model according to Equation 5.3b. In this case, f_{oc} is specified in the aquifer-specific input group according to Equation 5.2, and k_{oc} is a constituent-specific input value (see Section 3.3.2.1). However, if site-specific data are available, a constant value or distribution of values could be used for the leading Freundlich coefficient.

When modeling metals transport in the saturated zone with EPACMTP, the leading Freundlich coefficient can be specified as a constant value or as a distribution of values, either based on site-specific data or adsorption data reported in the scientific literature. Another option is to specify sorption according to equations comprising *pH*-based (linear) isotherms. In this case, this input parameter is not used; that is, this record in the input file is ignored by the model. Instead, the K_d^s (Equation 5.3c) is calculated as a function of *pH* (see Section 3.3.3.1.2).

Alternatively, if tables of non-linear sorption isotherms developed using the MINTEQA2 geochemical model are used to model transport in the unsaturated zone, then a single K_d^s value is chosen from these tabulated data to be used in the aquifer. As implemented in EPACMTP, the non-linearity of the isotherms is most important in the unsaturated zone where the concentrations are relatively high. Upon reaching the water table and mixing the leachate with ambient ground water, the metal's concentration is considered to be low enough that a linear isotherm can always be used. The appropriate saturated zone K_d^s value is automatically chosen by the model based on the maximum ground-water concentration under the source. In this case as well, this input parameter is not used; that is, this record in the input file is ignored by the model. Instead, the K_d^s (Equation 5.3c) is chosen from tabulated data (see Sections 3.3.3.2 and 5.3.13 and Appendix B).

Data Sources

Generally, the K_d^s for organic constituents is specified as a derived parameter; however, if this option is not appropriate and site-specific data are not available, there are studies in the scientific literature that provide compilations of K_d^s values that have been measured in the field (for instance, see *Risk Assessment for the Listing Determinations for Inorganic Chemical Manufacturing Wastes*; U.S. EPA, 2000). In this case, the leading Freundlich coefficient would be specified as either a constant value or a distribution of values (and the Freundlich exponent would be set to its default value of 1.0).

The leading Freundlich coefficient for metals is generally superseded by use of either the MINTEQA2-derived sorption data or the *pH*-based linear isotherms that were developed specifically for use with the EPACMTP model (see Section 3.3.3). However, if neither of these two options is appropriate and site-specific data are not available, there are studies in the scientific literature that provide compilations of K_d^s 's

that have been measured in the field (for instance, see Appendix I of U.S. EPA, 2000). In this case, the leading Freundlich coefficient would be specified as either a constant value or a distribution of values.

Use In EPACMTP

The leading Freundlich coefficient (also called the distribution coefficient) is one of the parameters used to calculate the amount by which contaminant transport is retarded relative to the ambient ground-water flow velocity within the aquifer. It is an input to the saturated zone transport module.

5.3.13 Exponent of Freundlich Isotherm for Saturated Zone (η^s)

Definition

The exponent of the Freundlich isotherm is a constant used to describe the sorptive behavior of a constituent. When the sorption data are plotted as $\log C$ versus $\log S$, the slope of the resulting line is equal to η^s . In the special case of a linear isotherm, the exponent of the Freundlich isotherm is equal to 1.0.

Parameter Value or Distribution of Values

For modeling organic constituents, the default value of the Freundlich exponent is 1.0, meaning a linear adsorption isotherm is used.

When modeling metals transport in the saturated zone with EPACMTP, the distribution coefficient for metals is generally specified using either tabulated non-linear MINTEQA2 isotherms or pH-based linear isotherms that were developed specifically for use with the EPACMTP model (see Section 3.3.3). In these two cases, the K_d data is either read in from an auxiliary input file or internally calculated, and the Freundlich isotherm coefficient and exponent are not used. If the leading Freundlich coefficient is specified using an empirical distribution of values (e.g., based on reported K_d values in the scientific literature), then the Freundlich isotherm exponent should be set equal to 1.0.

If this parameter is omitted from the data file, it is assigned a default value of 1.0, which is equivalent to specifying a linear sorption isotherm.

In EPACMTP Version 2.0, only the case of $\eta = 1$ is permitted. Non-linear isotherms (see Equation 5.3c) to describe metals transport are used only in the unsaturated zone and are handled using the tabular type of input described in Section 3.3.3.2 and Appendix B.

Data Sources

For modeling organic constituents, the Freundlich isotherm exponent is generally set to its default value of 1.0, and so no specific data source is used to determine the appropriate value for the Freundlich exponent.

For modeling metal constituents, the Freundlich isotherm exponent is not used as an input parameter, and so no specific data source is used (see Section 3.3.3.2). If literature or site-specific data are used to specify a non-linear adsorption isotherm, modeling of the adsorption process is implemented via tabular input describing the relationship in Equation 5.3c.

Use In EPACMTP

The Freundlich exponent is one of the parameters used to calculate the amount by which contaminant transport is retarded relative to the ambient ground-water flow velocity within the aquifer; it is an input to the saturated zone transport module.

5.3.14 Chemical Degradation Rate Coefficient for Saturated Zone (λ_c^s)**Definition**

EPACMTP accounts for all transformation processes (both biological and chemical) using a lumped first-order decay coefficient. This overall decay coefficient is the sum of the chemical and biological transformation coefficients. The chemical degradation coefficient for the saturated zone is simply the rate of decay that is caused by chemical reactions (usually hydrolysis) in the saturated zone.

Parameter Value or Distribution of Values

By default, the chemical degradation coefficient in the saturated zone is set to be internally derived using the hydrolysis rate constants and the saturated zone properties according to Equation 3.4. However, if site-specific data are available, this parameter can be specified as a constant value or a distribution of values. In this case, the hydrolysis rate constants can be omitted from the input file.

Data Sources

If this parameter is not derived by the model, then a site-specific data source must be used to determine the appropriate input value.

Use In EPACMTP

The chemical degradation coefficient is used by the model to calculate the amount by which ground-water concentrations are attenuated due to chemical hydrolysis; it is an input to the saturated zone transport module and is one of the

parameters required to solve the advection-dispersion equation (see Sections 3.3.4 and 4.4.4 of the *EPACMTP Technical Background Document* (U.S. EPA, 2003a).

5.3.15 Biodegradation Rate Coefficient for Saturated Zone (λ_b^s)

Definition

EPACMTP accounts for all transformation processes (both biological and chemical) using a lumped first-order decay coefficient. This overall decay coefficient is the sum of the chemical and biological transformation coefficients. The biological degradation coefficient for the saturated zone is simply the rate of decay that is caused by biological processes in the saturated zone.

Parameter Value or Distribution of Values

By default, the biological degradation coefficient in the saturated zone is set equal to zero. However, if site-specific data are available, this parameter can be specified as a constant value or a distribution of values.

Data Sources

If the input value of this parameter is non-zero, then a site-specific data source must be used to determine the appropriate input value.

Use In EPACMTP

The biological degradation coefficient is used by the model to calculate the amount by which ground-water concentrations are attenuated due to biological processes; it is an input to the saturated zone transport module and is one of the parameters required to solve the advection-dispersion equation (see Sections 3.3.4 and 4.4.4 of the *EPACMTP Technical Background Document* (U.S. EPA, 2003a).

6.0 RECEPTOR WELL PARAMETERS

A receptor well is a hypothetical drinking water well that is located downgradient of the waste management unit in consideration. It represents the location at which the potential exposure to the ground water is measured. Discussed in this section are the EPACMTP input parameters which govern the generation and constraining of the receptor well location. These include Monte Carlo parameters that the user can specify. These parameters can be used to apply (or not apply) particular constraints on parameter values or generation methodology.

6.1 RECEPTOR WELL PARAMETERS

The parameters listed below in Table 6.1 are used to define the characteristics of the downgradient receptor well.

Table 6.1 Receptor Well Parameters

Parameter	Symbol	Units	Section	Equation in EPACMTP TBD
Radial Distance to Receptor Well	R_{rw}	m	6.2	4.21, 4.22, 4.25 and 4.26
Angle of Well Off of Plume Centerline	θ_{rw}	degrees	6.3	4.26a
Downgradient Distance to Receptor Well	x_{rw}	m	6.4	4.21, 4.25a and 4.26b
Well Distance From Plume Centerline	y_{rw}	m	6.5	4.22, 4.25b and 4.26c
R_{rw} Origination Method	IWLOC	-	6.5	Section 4.4.3.6
Constraint on Well Distance From Plume Centerline	LYCHK	-	6.5	4.28 as constraint on y_{rw}
Depth of Intake Point Below Watertable	z_{rw}^*	m	6.6	4.29
Constraint on Depth of Intake Point Below Watertable	LZCHK	-	6.6	4.29 as constraint on z_{rw}^*
Averaging Period for Ground-water Concentration at Receptor Well	t_d	yr	6.7	4.108 and 4.109

EPACMTP ultimately represents the receptor well location in a Cartesian coordinate system whose X axis is oriented along the plume centerline for convenience. However, the user can specify the areal receptor well location in either cylindrical (R_{rw}, θ_{rw}) or Cartesian (x_{rw}, y_{rw}) coordinates and the model will transform the inputs accordingly. It's important to note that the specification of the receptor well

depth, z_{rw}^* , is not dependent upon the chosen coordinate system. Figure 6.1 illustrates how the receptor well location is determined using cylindrical coordinates (Figure 6.1a) and Cartesian coordinates (Figure 6.1b).

EPACMTP provides two optional constraints to force receptor well locations into the interior of the dissolved constituent plume; one constraint applies to the areal location of the receptor well (LYCHK), and the other constrains the depth of the receptor well (LZCHK). By default, the receptor well can be located anywhere downgradient of the WMU (radial distance of up to about one mile, with the angle off-center varying uniformly between 0 and 90 degrees) and anywhere within the saturated thickness of the aquifer.

An additional option (IWLOC) provides a receptor well locating methodology which addresses the tendency of WMUs with very large areas (e.g., LAUs) to bias upward the Monte Carlo receptor well concentrations. This option is further described in Section 6.5.

The final parameter discussed in this section is the averaging period for ground water concentration at the receptor well. The averaging period is useful for risk calculations which require an estimate of the exposure concentration over a period of time, say 30 years.

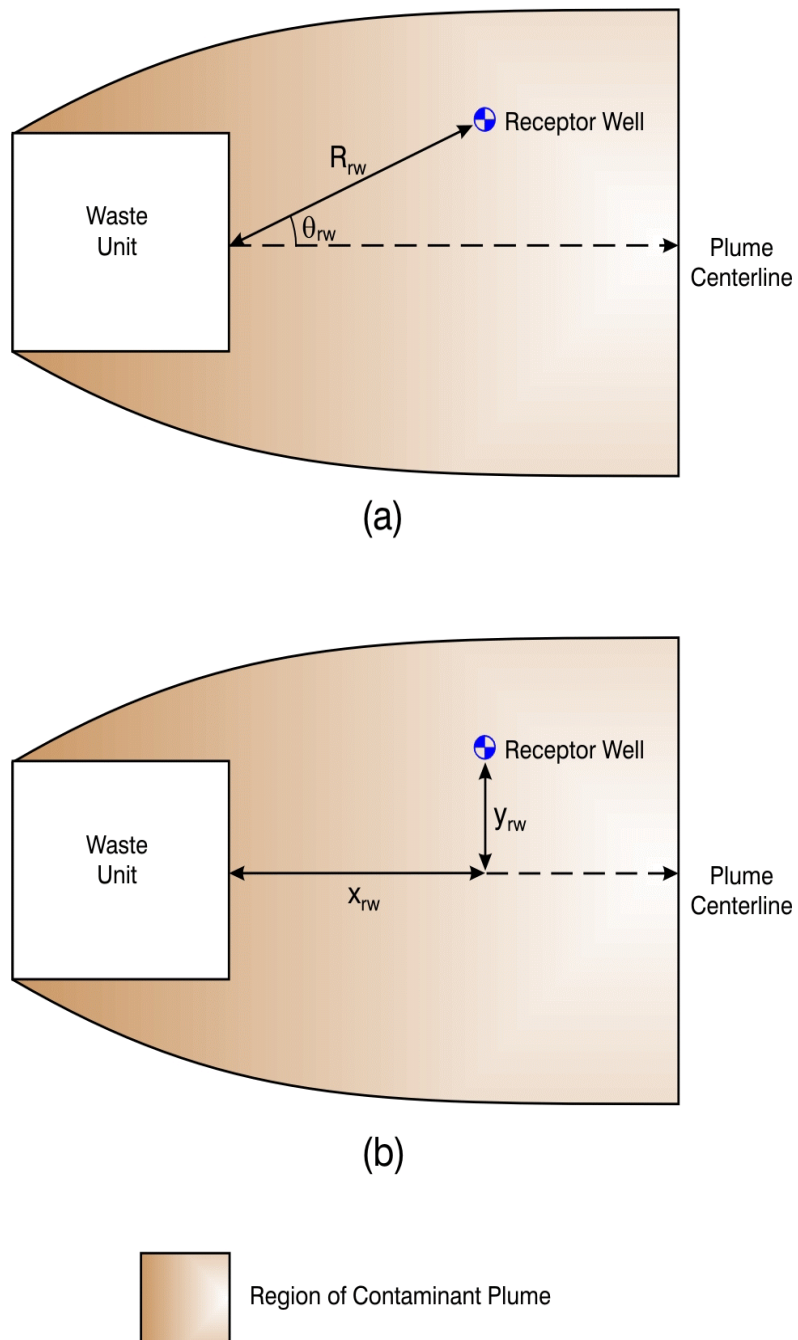


Figure 6.1 Schematic plan view showing procedure for determining the downstream location of the receptor well: (a) well location determined using radial distance, R_{rw} , and angle off center θ_{rw} ; and (b) well location generated uniformly within plume limit

6.2 RADIAL DISTANCE TO RECEPTOR WELL (R_{rw})

Definition

The radial distance to the receptor well (m) is measured from the downgradient edge of the WMU to the nearest downgradient receptor well, as depicted in Figure 6.1a.

Parameter Value or Distribution of Values

As shown in Figures 6.1a and 6.1b, the default reference point or origin for determining the receptor well location is midpoint of the downgradient edge of the WMU. EPACMTP provides an alternative receptor well location methodology for determining the reference point and it is controlled by the Monte Carlo control parameter IWLOC. Setting the Monte Carlo control parameter IWLOC equal to zero instructs EPACMTP to use the default reference point for determining the receptor well location. If IWLOC is set equal to one, the alternate location method is used. The alternate method has been included as a means to reduce the bias introduced by WMUs with large areas. When R_{rw} is always measured from the default reference point, receptor well locations are more likely to lay inside the areal extent of the dissolved constituent plume as the size of the WMU increases, biasing exposure concentrations upward. To reduce the potential bias, the reference point in the alternate scenario may be at any point somewhere between the corner and the center of the downgradient edge of the WMU. Section 4.4.3.6 in the *EPACMTP Technical Background Document* (U.S. EPA, 2003a) describes the alternate method in detail. R_{rw} may be specified by any appropriate distribution of values or by a constant value to accommodate site-specific data or analysis-specific assumptions. Lacking site-specific data, R_{rw} is typically determined using the empirical distribution shown in Table 6.2.

Data Sources

In a Monte Carlo simulation, the primary output from the model is the exposure concentration at a receptor well located downgradient from the waste site. Available studies and surveys suggest that on average, multiple downgradient wells are present within the one-mile distance that is typically considered in regulatory applications. To ensure a degree of protection in the modeling analysis, the model computes the concentration at the nearest downgradient well. Information on the downgradient distance to the nearest receptor well can be obtained from the U.S. EPA OSW landfill survey (U.S. EPA, 1993). These data are presented as an empirical distribution in Table 6.2. At most waste sites included in this survey, the direction of ambient ground-water flow was not known exactly; therefore, it cannot be ascertained whether the nearest receptor well is located directly along the plume centerline. To reflect uncertainties and variations in the location of the receptor well in relation to the direction of ambient ground-water flow, the modeled well is typically allowed to be positioned at some varying distance from the plume centerline.

Table 6.2 Cumulative Probability of Distance to Nearest Receptor Well for Landfills (from EPA, 1993)

Cumulative Probability	Radial Distance (m)
0.0	0.6
0.03	13.7
0.04	19.8
0.05	45.7
0.10	103.6
0.15	152.4
0.20	182.9
0.25	243.8
0.30	304.8
0.35	304.8
0.40	365.7
0.45	396.2
0.50	426.7
0.55	457.2
0.60	609.6
0.65	762.0
0.70	804.6
0.75	868.6
0.80	914.4
0.85	1158.2
0.90	1219.1
0.95	1371.5
0.98	1523.9
1.00	1609.3

Use In EPACMTP

The first, and default, option of determining the well location involves determining the Cartesian coordinates of the receptor well as a function of the radial distance (R_w) from the center of the downgradient edge of the WMU and the angle off of the plume centerline (θ_{rw}), as depicted in Figure 6.1a. If R_w is specified, θ_{rw} must also be specified. EPACMTP will derive x_{rw} and y_{rw} from the cylindrical coordinates (see Section 6.4).

6.3 ANGLE OF WELL OFF OF PLUME CENTERLINE (θ_{rw})

Definition

The first, and default, option of determining the well location involves determining the Cartesian coordinates of the receptor well as a function of the radial distance (R_w) from the center of the downgradient edge of the WMU and the angle

off of the plume centerline (θ_{rw}), as depicted in Figure 6.1a. This angle, in conjunction with R_{rw} , defines the receptor well location in the cylindrical coordinates.

Parameter Value or Distribution of Values

θ_{rw} may be specified by any appropriate distribution of values or by a constant value to accommodate site-specific data or analysis-specific assumptions. For example, setting θ_{rw} to zero would constrain the receptor well location to the plume centerline. Lacking site-specific data, to include all potential wells located downstream of the waste units, the angle θ_{rw} is typically taken to be uniformly distributed between 0° and 90° .

Data Sources

In a Monte Carlo simulation, the primary output from the model is the exposure concentration at receptor well located downgradient from the waste site. If site-specific data are unavailable, a default distribution of values may be used. Since multiple downgradient wells are often present within the default one-mile distance, to be protective, the modeled receptor well is taken to be the nearest downgradient well based on an EPA OSW survey of municipal landfills (U.S. EPA, 1993). However, at most waste sites included in this survey, the direction of ambient ground-water flow was not known exactly; therefore, it cannot be ascertained whether the nearest receptor well is located directly along the plume centerline. To reflect uncertainties and variations in the location of the receptor well in relation to the direction of ambient ground-water flow, the modeled well is typically allowed to be positioned at a variable y-distance from the plume centerline.

Thus, to include all hypothetical receptor wells located downstream of the waste units, the angle θ_{rw} is, by default, assumed to be uniformly distributed between 0° and 90° .

Use In EPACMTP

The first, and default, option of determining the well location involves determining the Cartesian coordinates of the receptor well as a function of the radial distance (R_{rw}) from the center of the downgradient edge of the WMU and the angle off of the plume centerline (θ_{rw}), as depicted in Figure 6.1a. If θ_{rw} is specified, R_{rw} must also be specified. EPACMTP will derive x_{rw} and y_{rw} from the cylindrical coordinates (see Section 6.4).

6.4 DOWNGRADIENT DISTANCE TO RECEPTOR WELL (x_{rw})

Definition

The downgradient distance to the receptor well (m) is the distance to the well, as measured from the center of downgradient edge of the WMU along the long-term average ground-water flow path (plume centerline), as depicted in Figure 6.1b.

Parameter Value or Distribution of Values

The first, and default, option of determining the well location involves determining the Cartesian coordinates of the receptor well as a function of the radial distance, R_{rw} , from the center of the downgradient edge of the waste unit, and the angle off-center, θ_{rw} , as depicted in Figure 6.1a. x_{rw} is derived using the following equation:

$$x_{rw} = R_{rw} \cos (\theta_{rw}) \quad (6.1)$$

where

x_{rw}	=	X Cartesian coordinate of the receptor well (m)
R_{rw}	=	radial distance between waste unit and well (m),
θ_{rw}	=	angle measured counter-clockwise from the plume centerline (degrees)

The second method incorporated in EPACMTP to determine the receptor well location is to generate a well position directly from the Cartesian coordinates, x_{rw} and y_{rw} . In this case, the Cartesian parameters are specified in the EPACMTP input file, and the cylindrical parameters are ignored (typically these inputs are omitted from the input file). If site-specific data on well location(s) are available, then these data can be used to specify a constant value or an empirical or statistical distribution of values for x_{rw} and y_{rw} .

Alternatively, x_{rw} and y_{rw} can also be used to specify the well location such that the well is located uniformly between the plume centerline and the areal plume boundary, for any given x-distance (Figure 6.1b). This option is described further in Section 6.5 (Well Distance From Plume Centerline (y_w)).

To reflect uncertainties and variations in the location of the receptor well in relation to the direction of ambient ground-water flow, the modeled well is allowed to be positioned at some varying distance from the plume centerline.

Data Sources

Lacking site-specific data, information on the downgradient distance to the nearest receptor well can be obtained from the U.S. EPA OSW landfill survey (U.S. EPA, 1993). These data are presented as an empirical distribution in Table 6.2.

Use In EPACMTP

The downgradient distance to the receptor well (x_{rw}) is used to represent the location at which the potential exposure concentration to the ground water is measured.

6.5 WELL DISTANCE FROM PLUME CENTERLINE (y_{rw})

Definition

The well distance from the plume centerline (m) is the distance from the plume centerline to the well, measured perpendicular to the plume centerline, as depicted in Figure 6.1b.

Parameter Value or Distribution of Values

The first, and default, option of determining the well location involves determining the Cartesian coordinates of the receptor well as a function of the radial distance, R_{rw} , from the center of the downgradient edge of the waste unit, and the angle off-center, θ_{rw} , as depicted in Figure 6.1a. The parameter y_{rw} is derived using the following equation:

$$y_{rw} = R_{rw} \sin (\theta_{rw}) \quad (6.2)$$

where

y_{rw}	=	Y Cartesian coordinate of the receptor well (m)
R_{rw}	=	radial distance between waste unit and well (m),
θ_{rw}	=	angle measured counter-clockwise from the plume centerline (degrees)

The second method incorporated in EPACMTP to determine the receptor well location is to generate a well position directly from the Cartesian coordinates, x_{rw} and y_{rw} . In this case, the Cartesian parameters are specified in the EPACMTP input file, and the cylindrical parameters are ignored (typically these inputs are omitted from the input file). If site-specific data on well location(s) are available, then these data can be used to specify a constant value or an empirical or statistical distribution of values for x_{rw} and y_{rw} .

Alternatively, x_{rw} and y_{rw} can also be used to estimate the well location such that the well is located uniformly between the plume centerline and the areal plume boundary, for any given x-distance (Figure 6.1b). With this option, x_{rw} is generated from the empirical distribution in Table 6.2. Next, the y_{rw} of the well is generated from a uniform distribution with a minimum value of zero, and a maximum value given by the following equation:

$$y_{rw} \leq y_D + 3[2\alpha_T(x_w + x_{rw})]^{1/2} \quad (6.3)$$

where

y_D	=	width of the waste unit in the y-direction (m)
x_{rw}	=	length of the waste unit in the x-direction (m)
α_T	=	horizontal transverse dispersivity (m)
x_w	=	length of the WMU in the x-direction (parallel to ground-water flow) (m)

This approximation for the lateral extent of the contaminant plume is based on the assumption that plume spreading in the horizontal-transverse direction is caused by dispersive mixing, which results in a Gaussian profile of the plume cross-section. Use of Equation 6-3 implies that 99.7% of the contaminant mass will be present inside the transverse plume limit.

To select this option, the Monte Carlo control parameter LYCHK should be set to TRUE, the x_{rw} should be specified as an empirical parameter with values as given in Table 6.2, and the y_{rw} should be specified as a uniform distribution with limits of zero and one.

Data Sources

No default data sources are available for y_{rw} . Information on the downstream distance to the nearest receptor well can be obtained from the U.S. EPA OSW landfill survey (U.S. EPA, 1993). These data are presented as an empirical distribution in Table 6.2. At most waste sites included in this survey, the direction of ambient ground-water flow was not known exactly; therefore, it cannot be ascertained whether the nearest receptor well is located directly along the plume centerline. To reflect uncertainties and variations in the location of the receptor well in relation to the direction of ambient ground-water flow, the modeled well is typically allowed to be positioned at some varying distance from the plume centerline if site-specific data are not available.

Use In EPACMTP

Along with the term x_{rw} (downgradient distance to the receptor well), the y_{rw} parameter is used to define the location of a receptor well. The y_{rw} parameter represents the perpendicular distance from the plume centerline at which the potential exposure to the ground water is measured. Setting y_{rw} to zero constrains the receptor well location to the plume centerline.

6.6 DEPTH OF INTAKE POINT BELOW WATERTABLE (z_{rw}^*)

Definition

The depth of the intake point below the water table (m) is the depth at which the model calculates the resulting ground-water concentration. Unlike most wells in the real world that have a screened interval of several feet or more, the simulated receptor well in EPACMTP has an intake that is a single point in space, as if the well consisted of a solid casing that was open at the bottom. In this case, the intake point would be the same as the depth of the well (or z_{rw}^*). Note that this depth is measured downwards from the watertable, not from the ground surface.

Parameter Value or Distribution of Values

Three options are available for specifying the vertical position of the well intake point below the water table: uniform distribution, constrained distribution, or constant value.

The first, and default, option is to model the vertical position of the well intake point as being uniformly distributed between the water table ($z=0$) and the saturated aquifer thickness. This option is selected by specifying the z -position as a uniform distribution with lower and upper limits of 0.0 and 1.0. EPACMTP will multiply this uniformly generated value by the saturated zone thickness to yield the actual receptor well depth below the water table for each Monte Carlo iteration. When the generated value for the vertical position of the receptor well intake point exceeds the saturated thickness of the aquifer (a physically impossible condition), a new well position is generated to ensure that the well depth is always less than the saturated thickness. Conversely, the well depth cannot be less than the minimum depth to the saturated zone.

Alternatively, the vertical position of the observation well can be optionally constrained to lie within the approximate vertical penetration depth of the contaminant plume emanating from the waste unit. This is achieved through the Monte Carlo input variable LZCHK. If LZCHK is set to FALSE, the constraint is not enforced. If LZCHK is set to TRUE, the z_{rw}^* is constrained to lie within the approximate vertical extent of the contaminant plume as defined by:

$$z_{rw}^* \leq 2.5 \left\{ \frac{Q_3^F + Q_4^F}{Q_1^F} B + \left[\alpha_v (x_w + x_{rw}) + \alpha_L \left(\frac{Q_3^F + Q_4^F}{Q_1^F} B \right) + \phi_e D^{s*} \right]^{\frac{1}{2}} \right\} = z_{rw}^* \max \quad (6.4)$$

where

$z_{rw\ max}^*$	=	Maximum allowable z^* -coordinate of the receptor well; that is, the approximate vertical penetration depth of the dissolved constituent plume (m)
$Q_1^F - Q_4^F$	=	Components of the ground-water flow field (m^2/yr), see U.S. EPA (2003a), Section 4, Figure 4.7
B	=	Saturated zone thickness (m)
x_w	=	Length of source in downstream direction (m)
x_{rw}	=	Horizontal distance between source and receptor well (m)
α_L	=	Longitudinal dispersivity (m)
α_v	=	Vertical dispersivity (m)
ϕ_e	=	Effective porosity of the aquifer (dimensionless)
D^s	=	Effective molecular diffusion coefficient (m^2/y)

As a third option, the well position may be fixed at a constant absolute depth or as a constant relative depth (as a constant fractional depth of the saturated thickness).

Data Sources

In the absence of site-specific data for this input, z_{rw}^* is typically defined as a uniformly distributed fraction of the saturated thickness.

Use In EPACMTP

The depth of the intake point below the water table is the depth at which the model calculates the resulting ground-water concentration. It is from this point that a ground-water concentration of a potential contaminant plume would be established.

6.7 AVERAGING PERIOD FOR GROUND-WATER CONCENTRATION AT RECEPTOR WELL (t_d)

Definition

The averaging period for the ground-water concentration at the receptor well (yr) is the time period over which the average concentration is calculated. For instance, if this input is specified as 30 years, then the EPACMTP model would search for the highest 30-year average concentration over the specified modeling period and report this concentration in the output file. This ground-water averaging time should correspond to the exposure duration used in the health-risk calculations for carcinogenic constituents. Up to ten averaging times may be specified.

Parameter Value or Distribution of Values

Usual values of this parameter are 70 years (lifetime exposure), 30 years (high-end residence time), 9 years (average residence time), or 7 years (child exposure) (U.S. EPA, 2000). Although this value is often entered as a constant value, it can also be specified as a statistical or empirical distribution of values.

By default, the exposure period for averaging the receptor well concentration is not provided; in other words, the model only calculates the peak receptor well concentration. The peak receptor well concentration is sometimes used for calculating the resulting health risk for non-carcinogenic constituents or for comparisons to the maximum contaminant levels (MCLs) (The National Drinking Water Standards at 40 CFR 141).

Data Sources

The choice of the averaging period should be consistent with the types of risks to be calculated using the exposure results generated by EPACMTP. The EPA's *Exposure Factors Handbook* (U.S. EPA 1997a-c) contains constituent-specific data on exposure durations for various exposure scenarios.

Use In EPACMTP

EPACMTP always generates a steady state receptor well concentration and a peak concentration. Steady state concentrations correspond to an infinite source analysis; peak concentrations represent the maximum concentration at the well under the finite source scenario. Average concentrations for defined exposure periods are optional results for finite source simulations. If average concentrations are required, up to 10 averaging periods can be specified. If the period of averaging is longer than the period of time for which concentrations are observed at the receptor well, the result will be the average of the available observations.

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